10/552,595K Yong Chu 12/17/2009

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptaylc1626

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	AUG 10	Time limit for inactive STN sessions doubles to 40 minutes
NEWS 3	AUG 18	COMPENDEX indexing changed for the Corporate Source (CS) field
NEWS 4	AUG 24	ENCOMPLIT/ENCOMPLIT2 reloaded and enhanced
NEWS 5	AUG 24	CA/CAplus enhanced with legal status information for U.S. patents
NEWS 6	SEP 09	50 Millionth Unique Chemical Substance Recorded in CAS REGISTRY
NEWS 7	SEP 11	WPIDS, WPINDEX, and WPIX now include Japanese FTERM thesaurus
NEWS 8	OCT 21	Derwent World Patents Index Coverage of Indian and Taiwanese Content Expanded
NEWS 9	OCT 21	Derwent World Patents Index enhanced with human translated claims for Chinese Applications and Utility Models
NEWS 10	NOV 23	Addition of SCAN format to selected STN databases
NEWS 11	NOV 23	Annual Reload of IFI Databases
NEWS 12	DEC 01	FRFULL Content and Search Enhancements
NEWS 13	DEC 01	DGENE, USGENE, and PCTGEN: new percent identity feature for sorting BLAST answer sets
NEWS 14	DEC 02	Derwent World Patent Index: Japanese FI-TERM thesaurus added
NEWS 15	DEC 02	PCTGEN enhanced with patent family and legal status display data from INPADOCDB
NEWS 16	DEC 02	USGENE: Enhanced coverage of bibliographic and sequence information

NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that specific topic.

and other penalties.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:50:08 ON 17 DEC 2009

=> file reg
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 0.22 0.22

FILE 'REGISTRY' ENTERED AT 10:50:32 ON 17 DEC 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 15 DEC 2009 HIGHEST RN 1197459-30-5
DICTIONARY FILE UPDATES: 15 DEC 2009 HIGHEST RN 1197459-30-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and
Settings\ychu\Desktop\Case\10552595\10552595K_12172009.str

full scope

chain nodes :
21 23

```
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16
chain bonds :
4-21
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-11  8-9  9-10  10-11  12-13  12-16  13-14  14-
15
15-16
exact/norm bonds :
4-21  7-8  7-11  8-9  9-10  10-11  12-13  12-16  13-14  14-15  15-16
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6
isolated ring systems :
containing 1 : 7 : 12 :


G1:[*1],[*2]

G2:H,O,S,N,X,Ak,CN,NO2

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  21:CLASS  23:CLASS  24:Atom




L1      STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l1
SAMPLE SEARCH INITIATED 10:51:01 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    40190 TO ITERATE

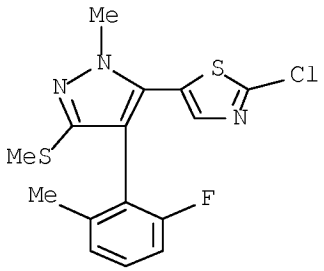
  5.0% PROCESSED     2000 ITERATIONS                                50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**      **too broad**
PROJECTED ITERATIONS:       791815 TO   815785
PROJECTED ANSWERS:          346500 TO   362450

L2           50 SEA SSS SAM L1

=> d scan

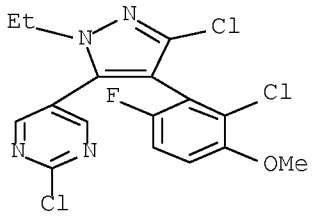
L2   50 ANSWERS   REGISTRY  COPYRIGHT 2009 ACS on STN
IN   Thiazole, 2-chloro-5-[4-(2-fluoro-6-methylphenyl)-1-methyl-3-(methylthio)-
     1H-pyrazol-5-yl]-
MF   C15 H13 Cl F N3 S2
```



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 50 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Pyrimidine, 2-chloro-5-[3-chloro-4-(2-chloro-6-fluoro-3-methoxyphenyl)-1-ethyl-1H-pyrazol-5-yl]-
MF C16 H12 Cl3 F N4 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> s l1 full
FULL SEARCH INITIATED 10:51:54 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 803163 TO ITERATE

78.6% PROCESSED 631026 ITERATIONS 272892 ANSWERS

90.2% PROCESSED 724100 ITERATIONS 316850 ANSWERS

100.0% PROCESSED 803163 ITERATIONS 364158 ANSWERS
SEARCH TIME: 00.00.50

L3 364158 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	187.32	187.54

FILE 'CAPLUS' ENTERED AT 10:53:00 ON 17 DEC 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 17 Dec 2009 VOL 151 ISS 25
FILE LAST UPDATED: 16 Dec 2009 (20091216/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2009

CAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
TOO MANY TERMS FOR FILE CROSSOVER IN L3
There are limits on the size of an answer set being crossed over from one file to another. Enter HELP CROSSOVER at an arrow prompt (=>) for specific information.

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.50	188.04

FILE 'REGISTRY' ENTERED AT 10:53:14 ON 17 DEC 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 DEC 2009 HIGHEST RN 1197459-30-5
DICTIONARY FILE UPDATES: 15 DEC 2009 HIGHEST RN 1197459-30-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

```
  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> save l3
ENTER NAME OR (END):yc10552595K/a
SAVED ANSWER LIMIT HAS BEEN REACHED
SAVE COMMAND INCOMPLETE

  The SAVE command did not complete successfully. Please find the
  preceding message text below to identify the system limit that
  was reached:

  SAVED QUERY LIMIT HAS BEEN REACHED - the limit for the number of
  saved queries has been reached for this loginid.

  SAVED ANSWER SET LIMIT HAS BEEN REACHED - the limit for the number
  of saved answer sets has been reached for this loginid.

  SAVED ANSWER LIMIT HAS BEEN REACHED - the limit for the total number
  of answers for all saved answer sets has been reached for this
  loginid.

  SAVED TEMPORARY ANSWER LIMIT HAS BEEN REACHED - the limit for the
  total number of answers for all saved temporary answer sets has
  been reached for this loginid.

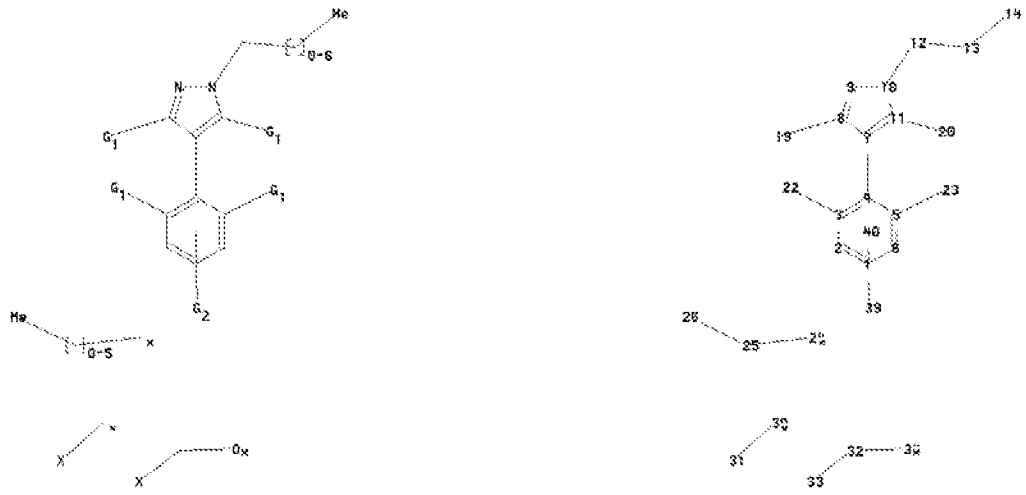
  SAVED L# LIST LIMIT HAS BEEN REACHED - the limit for the number of
  saved L# lists has been reached for this loginid.

  In all cases, use the DELETE command to delete the appropriate type
  of saved entities which are no longer needed and re-issue the SAVE
  command.

=> save l3 temp
ENTER NAME OR (END):10552595K/a
10552595K/A IS NOT A VALID SAVED NAME
Enter the name you wish to use for the saved query,
answer set, or L-number list.  The name must:
  1. Begin with a letter,
  2. Have 1-12 characters,
  3. Contain only letters (A-Z) and numbers (0-9),
  4. End with /Q for a query (search profile,
     structure, or screen set), /A for an answer
     set, or /L for an L-number list.
  5. Not already be in use as a saved name,
  6. Not be END, SAV, SAVE, SAVED
  7. Not have the form of an L-number (Lnnn).
ENTER NAME OR (END):YC10552595K/a
ANSWER SET L3 HAS BEEN SAVED AS 'YC10552595K/A'

=>
=>
```

Uploading C:\Documents and Settings\ychu\Desktop\Case\10552595\L21_12172009.str



chain nodes :
12 13 14 19 20 22 23 24 25 26 30 31 32 33 34 39
ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
3-22 4-7 5-23 8-19 10-12 11-20 12-13 13-14 24-25 25-26 30-31 32-33 32-34

ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11
exact/norm bonds :
3-22 5-23 8-9 8-19 9-10 10-11 10-12 11-20 32-34
exact bonds :
4-7 7-8 7-11 12-13 13-14 24-25 25-26 30-31 32-33
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 : 7 :

G1:H,CH3

G2:H,CH3,t-Bu,OH,SH,CN,NH,X

Hydrogen count :
12:>= minimum 1
Connectivity :
24:3 X maximum RC ring/chain 25:3 X maximum RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 13:CLASS 14:CLASS 19:CLASS 20:CLASS 22:CLASS 23:CLASS
24:CLASS 25:CLASS
26:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 39:CLASS 40:Atom

```
L4      STRUCTURE UPLOADED

=> d
L4 HAS NO ANSWERS
L4              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l4 sam sss sub=l3
SAMPLE SUBSET SEARCH INITIATED 11:25:52 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED -       31 TO ITERATE

100.0% PROCESSED       31 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET):           ONLINE  **COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET):          286 TO      954
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET):               0 TO        0

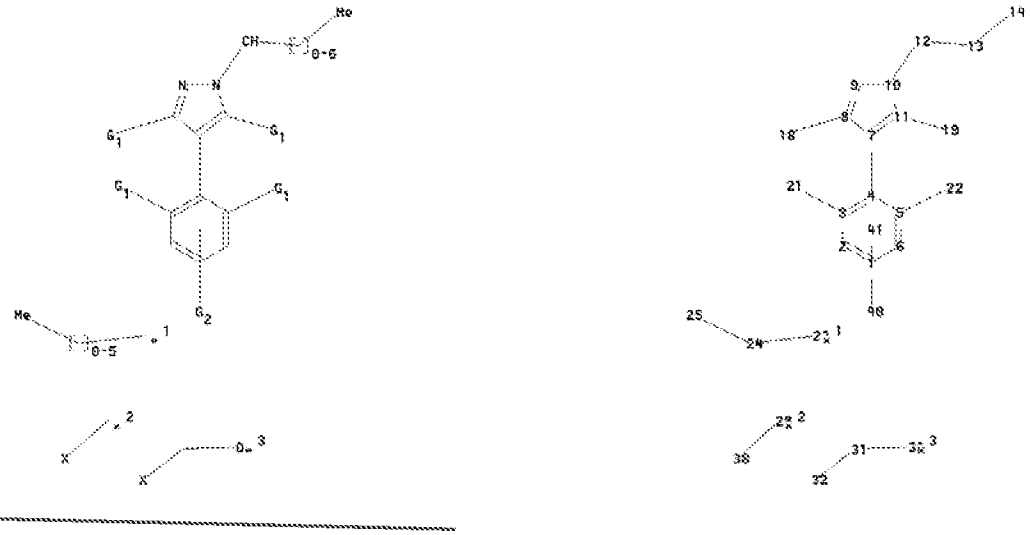
L5            0 SEA SUB=L3 SSS SAM L4

=> s l4 full sss sub=l3
FULL SUBSET SEARCH INITIATED 11:26:13 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -      757 TO ITERATE

100.0% PROCESSED      757 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

L6            0 SEA SUB=L3 SSS FUL L4

=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10552595\L22_12172009.str
```



```
chain nodes :
12  13  14  18  19  21  22  23  24  25  29  30  31  32  33  40
ring nodes :
```

```
1  2  3  4  5  6  7  8  9  10  11
chain bonds :
3-21  4-7  5-22  8-18  10-12  11-19  12-13  13-14  23-24  24-25  29-30  31-32  31-
33

ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-11  8-9  9-10  10-11
exact/norm bonds :
3-21  5-22  8-9  8-18  9-10  10-11  10-12  11-19  31-33
exact bonds :
4-7  7-8  7-11  12-13  13-14  23-24  24-25  29-30  31-32
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6
isolated ring systems :
containing 1 : 7 :


G1:H,CH3

G2:H,CH3,t-Bu,OH,SH,CN,NH,X,[*1],[*2],[*3]

Connectivity :
23:3 X maximum RC ring/chain
Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:CLASS  13:CLASS  14:CLASS  18:CLASS  19:CLASS  21:CLASS  22:CLASS
23:CLASS  24:CLASS
25:CLASS  29:CLASS  30:CLASS  31:CLASS  32:CLASS  33:CLASS  40:CLASS  41:Atom




L7      STRUCTURE UPLOADED

=> d
L7 HAS NO ANSWERS
L7              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l7 sam sss sub=l3
SAMPLE SUBSET SEARCH INITIATED 11:29:50 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED -      620 TO ITERATE

100.0% PROCESSED      620 ITERATIONS                            15 ANSWERS
SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET):           ONLINE  **COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET):        10907 TO    13893
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET):              68 TO      532

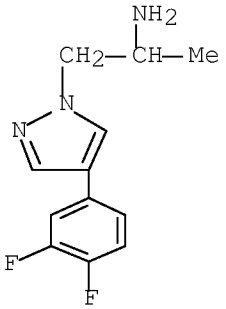
L8           15 SEA SUB=L3 SSS SAM L7

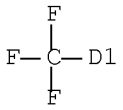
=> d scan

L8   15 ANSWERS   REGISTRY  COPYRIGHT 2009 ACS on STN
IN   1H-Pyrazole-1-ethanamine, 4-(3,4-difluorophenyl)-.alpha.,3(or
```

.alpha.,5)-dimethyl-5(or 3)-(trifluoromethyl)-, (.alpha.S)-
MF C14 H14 F5 N3
CI IDS

PAGE 1-A





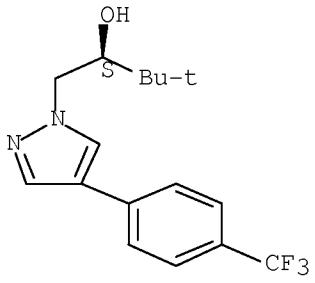
PAGE 2-A

D1—Me

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

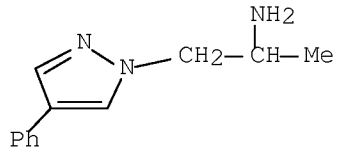
L8 15 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1H-Pyrazole-1-ethanol, .alpha.-(1,1-dimethylethyl)-4-[4-(trifluoromethyl)phenyl]-, (.alpha.S)-
MF C16 H19 F3 N2 O

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 15 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1H-Pyrazole-1-ethanamine, 3(or 5)-chloro-.alpha.-methyl-5(or 3)-(methylthio)-4-phenyl-, (.alpha.S)-
MF C13 H16 Cl N3 S
CI IDS



D1—S—Me

D1—Cl

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> s l7 full sss sub=l3
FULL SUBSET SEARCH INITIATED 11:30:49 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 11953 TO ITERATE

100.0% PROCESSED 11953 ITERATIONS 268 ANSWERS
SEARCH TIME: 00.00.01

L9 268 SEA SUB=L3 SSS FUL L7

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 118.24 306.28

FILE 'CAPLUS' ENTERED AT 11:30:55 ON 17 DEC 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 17 Dec 2009 VOL 151 ISS 25
FILE LAST UPDATED: 16 Dec 2009 (20091216/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2009

CAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l9
L10 57 L9 **Too many hits**

=> save l10 temp
ENTER NAME OR (END):yc10552595M/a
ANSWER SET L10 HAS BEEN SAVED AS 'YC10552595M/A'

=> file reg
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 3.50 309.78

FILE 'REGISTRY' ENTERED AT 11:34:51 ON 17 DEC 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 15 DEC 2009 HIGHEST RN 1197459-30-5
DICTIONARY FILE UPDATES: 15 DEC 2009 HIGHEST RN 1197459-30-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

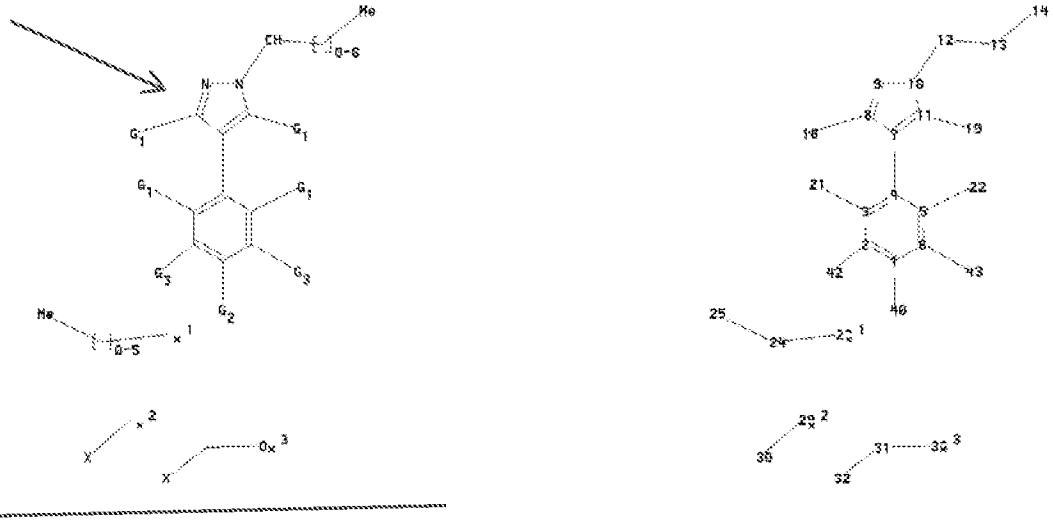
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10552595\L23_12172009.str

Searched scope



chain nodes :
12 13 14 18 19 21 22 23 24 25 29 30 31 32 33 40 42 43
ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
1-40 2-42 3-21 4-7 5-22 6-43 8-18 10-12 11-19 12-13 13-14 23-24 24-25
29-30 31-32 31-33
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11
exact/norm bonds :
1-40 2-42 3-21 5-22 6-43 8-9 8-18 9-10 10-11 10-12 11-19 31-33
exact bonds :
4-7 7-8 7-11 12-13 13-14 23-24 24-25 29-30 31-32
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 : 7 :

G1:H,CH3

G2:H,CH3,t-Bu,OH,SH,CN,NH,X,[*1],[*2],[*3]

G3:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Connectivity :
23:3 X maximum RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 13:CLASS 14:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS
23:CLASS 24:CLASS
25:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 40:CLASS 42:CLASS
43:CLASS

L11 STRUCTURE UPLOADED

```
=> d
L11 HAS NO ANSWERS
L11             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l11 sam sss sub=l3
SAMPLE SUBSET SEARCH INITIATED 11:35:26 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED -      620 TO ITERATE

100.0% PROCESSED      620 ITERATIONS                                4 ANSWERS
SEARCH TIME: 00.00.01

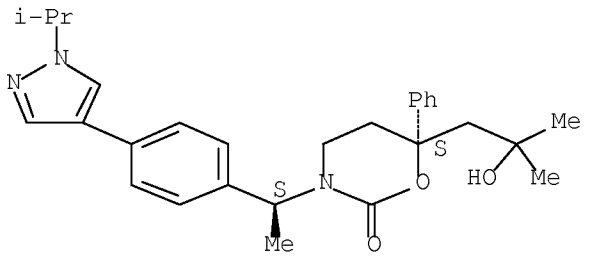
PROJECTIONS (WITHIN SPECIFIED SUBSET):           ONLINE  **COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET):        10907 TO    13893
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET):               4 TO      200

L12           4 SEA SUB=L3 SSS SAM L11

=> d scan

L12  4 ANSWERS   REGISTRY  COPYRIGHT 2009 ACS on STN
IN   INDEX NAME NOT YET ASSIGNED
MF   C28 H35 N3 O3

Absolute stereochemistry.
```




```
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> s l11 full sss sub=l3
FULL SUBSET SEARCH INITIATED 11:38:00 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -    11953 TO ITERATE

100.0% PROCESSED    11953 ITERATIONS                              49 ANSWERS
SEARCH TIME: 00.00.02

L13          49 SEA SUB=L3 SSS FUL L11

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
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	ENTRY	SESSION
FULL ESTIMATED COST	46.40	356.18

FILE 'CAPLUS' ENTERED AT 11:38:07 ON 17 DEC 2009
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FILE COVERS 1907 - 17 Dec 2009 VOL 151 ISS 25
FILE LAST UPDATED: 16 Dec 2009 (20091216/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2009

CAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

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=> s l13
L14 22 L13

=> d ibib abs hitstr tot
THE ESTIMATED COST FOR THIS REQUEST IS 124.08 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L14 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2009:1363231 CAPLUS Full-text
DOCUMENT NUMBER: 151:528776
TITLE: Oxazin-2-one compounds as inhibitors of 11beta-hydroxysteroid dehydrogenase 1 and their preparation, pharmaceutical compositions and use in the treatment of diseases
INVENTOR(S): Claremon, David A.; Zhuang, Linghang; Leftheris, Katerina; Tice, Colin M.; Xu, Zhenrong; Ye, Yuanjie; Singh, Suresh B.; Cacatian, Salvacion; Zhao, Wei; Himmelsbach, Frank; Eckhardt, Matthias
PATENT ASSIGNEE(S): Vitae Pharmaceuticals, Inc., USA; Boehringer Ingelheim International GmbH
SOURCE: PCT Int. Appl., 332pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2009134392	A1	20091105	WO 2009-US2641	20090430

W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

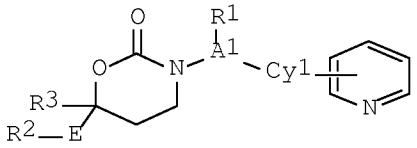
WO 2009017664	A1	20090205	WO 2008-US9017	20080725

W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.:		
US 2008-49650P	P	20080501
US 2008-137148P	P	20080725
WO 2008-US9017	A	20080725
US 2009-206775P	P	20090204
US 2007-962058P	P	20070726
US 2007-1253P	P	20071031

GI



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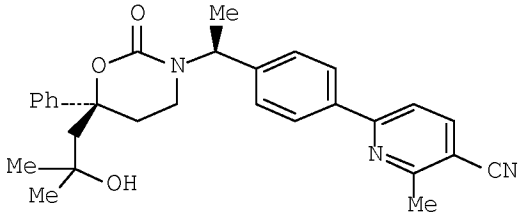


II

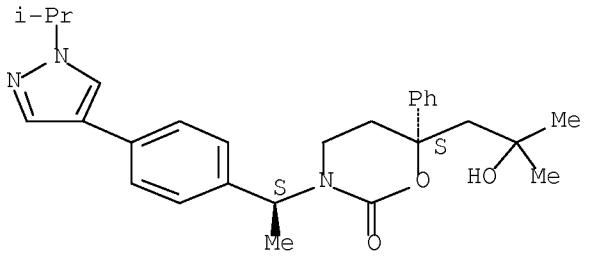
AB This invention relates to compds. of formula I pharmaceutically acceptable salts thereof, and pharmaceutical compns. thereof, which are useful for the therapeutic treatment of diseases assocd. with the modulation or inhibition of

11.beta.-HSD1 in mammals. Compds. of formula I wherein R1 is absent, (un)substituted C1-6 alkyl, (un)substituted C2-6 alkenyl, (un)substituted C2-6 alkynyl, etc.; A1 is a bond, C1-3 alkylene, CH2CH2O, and CH2CO; Cy1 is (un)substituted aryl, (un)substituted heteroaryl, (un)substituted monocyclic cycloalkyl and (un)substituted monocyclic heterocyclyl; E is a bond, (un)substituted C1-3 alkylene, and (un)substituted C1-2 alkenyleneoxy; R2 is (un)substituted C1-6 alkyl, (un)substituted aryl, (un)substituted heteroaryl, (un)substituted cycloalkyl and (un)substituted heterocyclyl; R3 is (un)substituted C1-6 alkyl, (un)substituted C2-6 alkylene, (un)substituted C2-6 alkynyl, etc.; and pharmaceutically acceptable salts, enantiomers, and diastereoisomers thereof, are claimed. Example compd. II was prepd. by bromination of 6-amino-2-methylnicotinonitrile; the resulting 6-bromo-2-methylnicotinonitrile underwent cross-coupling with (S)-6-(2-hydroxy-2-methylpropyl)-6-phenyl-3((S)-1-(4-(4,4,5,5-tetramethyl- 1,3,2-dioxaborolan-2-yl)phenyl)ethyl)-1,3-oxazin-2-one to give compd. II. All the invention compds. were evaluated for their 11.beta.-HSD1 inhibitory activity. From the assay, it was detd. that compd. II exhibited IC50 value of <100 nM and the av. inhibition at 100 nM was 96.4 %.

IT 1193244-69-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of oxazinone derivs. as inhibitors of 11beta-hydroxysteroid dehydrogenase 1 useful in the treatment of 11.beta.-HSD1-assocd. diseases)

RN 1193244-69-7 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2009:1262365 CAPLUS Full-text
DOCUMENT NUMBER: 151:470210
TITLE: Preparation of oxadiazolylphenylboronic acid derivatives and analogs for use as fatty acid amide hydrolase inhibitors
INVENTOR(S): Behnke, Mark L.; Castro, Alfredo C.; Evans, Catherine A.; Grenier, Louis; Grogan, Michael J.; Liu, Tao; Snyder, Daniel A.; Tibbitts, Thomas T.
PATENT ASSIGNEE(S): Infinity Pharmaceuticals, Inc, USA
SOURCE: PCT Int. Appl., 327pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

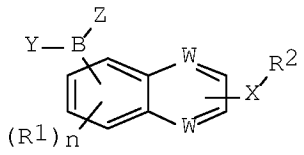
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2009126691	A1	20091015	WO 2009-US39872	20090408

W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2008-43686P P 20080409
OTHER SOURCE(S): MARPAT 151:470210
GI



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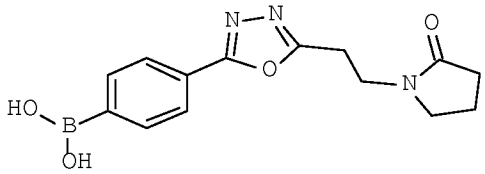


II

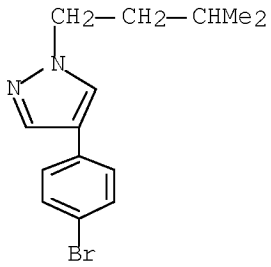
AB Title compds. I [each W independently = C, N, or CR12; X = covalent bond, O, S, C(O), etc.; Y = OH, OR3, (un)substituted alkyl, etc.; Z = OH or OR3; or Y and Z are taken together with the boron to which they are attached to form a ring contg. at least one O, S, N, or NR5 atom directly bonded to the boron atom; each R1 independently = halo, CF3, CN, NO2, etc.; R2 = H, halo, N3, CN, etc.; each R3 independently = (un)substituted alkyl, heteroalkyl, heterocyclyl, etc.; R5 = H, (un)substituted alkyl, heteroaryl, etc.; R12 = H, halo, CF3, etc.], and their pharmaceutically acceptable salts, are prepd. and disclosed as fatty acid amide hydrolase (FAAH) inhibitors. Thus, e.g., II was prepd. by cyclization of 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzohydrazine with 3-(2-oxopyrrolidin-1-yl)propionic acid followed by

hydrolysis. I were evaluated in human FAAH inhibition assays, e.g., II demonstrated a Ki value of 0.1 to 1 .mu.M.

IT 1191063-21-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of oxadiazolylphenylboronic acid derivs. and analogs for use as fatty acid amide hydrolase inhibitors)

RN 1191063-21-4 CAPLUS

CN 1H-Pyrazole, 4-(4-bromophenyl)-1-(3-methylbutyl)- (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2009:1010091 CAPLUS Full-text

DOCUMENT NUMBER: 151:288819

TITLE: Preparation of N-benzyl arylcarboxamide derivatives as glycine transporter inhibitors

INVENTOR(S): Yasuhara, Akitaka; Abe, Kimiyoshi; Yamamoto, Shuji; Shibata, Takeshi; Okubo, Taketoshi

PATENT ASSIGNEE(S): Taisho Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 42pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

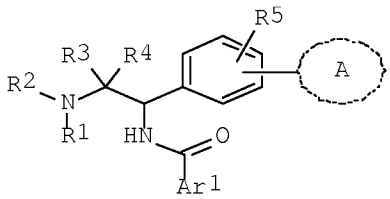
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2009185008	A	20090820	JP 2008-29617	20080208

PRIORITY APPLN. INFO.: JP 2008-29617 20080208

OTHER SOURCE(S): MARPAT 151:288819

GI



I

AB Title compds. I [ring A = Ph, naphthyl, monocyclic or dicyclic aryl contg. 1-2 heteroatom selected from N, O, and S, which may be optionally substituted with given substituents; Ar1 = any group given for A which may be substituted with given substituents; R1, R2 = H, (un)substituted C1-6 alkyl, (un)substituted C2-6 alkenyl, C3-8 cycloalkyl; Y = C1-6 alkyl, C3-8 cycloalkyl, halo, OH, C6-10 aryl, etc.; R3, R4 = H, halo, (un)substituted C1-6 alkyl, etc.; X = halo, OH, C1-6 alkoxy, etc.; n = 0-2; R5 = H, C1-6 alkyl, halo], their pharmaceutically-acceptable salts, or their hydrates inhibit glycine transporters and are useful for prevention or treatment of schizophrenia, Alzheimer disease, cognitive dysfunction, dementia, anxiety disorders, depression, drug dependence, convulsion, tremor, and/or sleep disorders. Thus, 2-chloro-N-[[4-(dimethylamino)-1,1-dioxidotetrahydro-2H- thiopyran-4-yl][3-(1-ethyl-1H-pyrazol-4-yl)phenyl]methyl]-3- (trifluoromethyl)benzamide (prepn. give) inhibited glycine uptake by human glycine transporter type 1 expressed on T98G glioma cells with IC50 20 nM.

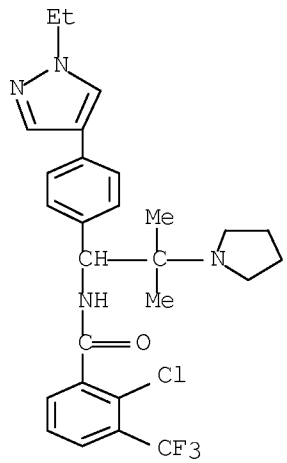
IT 1182296-73-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of N-benzyl arylcarboxamide derivs. as glycine transporter inhibitors)

RN 1182296-73-6 CAPLUS

CN Benzamide, 2-chloro-N-[1-[4-(1-ethyl-1H-pyrazol-4-yl)phenyl]-2-methyl-2-(1-pyrrolidinyl)propyl]-3-(trifluoromethyl)- (CA INDEX NAME)



L14 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2009:946270 CAPLUS Full-text

DOCUMENT NUMBER: 151:245363

TITLE: Preparation of biaryl derivatives as anticancer agents

INVENTOR(S): Asai, Akira; Sawada, Junichi; Matsuno, Kenji; Ogo, Naohisa; Nishigaki, Junji; Kojima, Masayoshi

PATENT ASSIGNEE(S): Pharma IP Limited Liability Intermediary Corporations, Japan

SOURCE: PCT Int. Appl., 135pp.
CODEN: PIXXD2

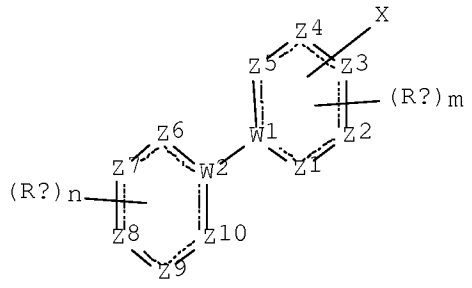
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2009096198	A1	20090806	WO 2009-JP395	20090202

W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: JP 2008-22504 A 20080201
OTHER SOURCE(S): MARPAT 151:245363
GI

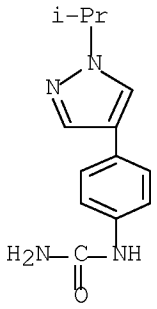


I

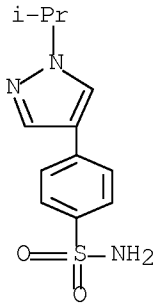
AB The title compds. I [W1, W2 is C=, N; at least one of Z1-Z10 is =N-, the others are =CH-; or two of Z1-Z10 which are adjacent to one another together represent NR1, O, S, Se; R1 = H, (un)substituted alkyl, (un)substituted alkenyl, etc.; X = -V-N(R2)-C(=Q1)-Y1, -V-N(R2)-S(O)p-Y2, -V-S(O)p-NR4R5; V = bond, (un)substituted alkylene; Q1 = O, S, CHNO2, etc.; Y1 = NR4R5, OR9, SR10; R4, R5 = H, (un)substituted alkyl, (un)substituted alkenyl, etc.; R9 = as defined for R1; R10 = as defined for R1; R2 = as defined for R1; Y2 = (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkynyl, etc.; p = 1 or 2; m = integer from 0 to 4; n = integer from 0 to 5; a proviso related to Z1-Z10 is given; Ra, Rb = (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkynyl, etc.; further details on Ra and Rb are given] are prepd. A mixt. of chlorosulfonyl isocyanate and tert-butanol in methylene chloride was stirred ; 2-amino-5-(4-tert-butylphenyl)pyridine and triethylamine were added to said mixt.; the reaction mixt. was stirred overnight to give, after workup, N'-tert-butoxycarbonyl-N-[5-(4-tert-butylphenyl)-2-pyridyl]sulfamide. In a test using HeLa cancer cells, compds. of this invention at 200 .mu.mol/L gave 52% to 98% inhibition of cell growth.

IT 1176725-38-4P 1176725-39-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(prepn. of biaryl derivs. as anticancer agents)
RN 1176725-38-4 CAPLUS
CN Urea, N-[4-[1-(1-methylethyl)-1H-pyrazol-4-yl]phenyl]- (CA INDEX NAME)



RN 1176725-39-5 CAPLUS
CN Benzenesulfonamide, 4-[1-(1-methylethyl)-1H-pyrazol-4-yl]- (CA INDEX NAME)



REFERENCE COUNT: 95 THERE ARE 95 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 5 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2009:739301 CAPLUS Full-text
DOCUMENT NUMBER: 151:77918
TITLE: Preparation of N-[4-(pyridin-4-yl)phenyl] amides as .gamma.-secretase modulators
INVENTOR(S): Hitchcock, Stephen; Chen, Jian J.; Ncube, Mqhele; Nixey, Thomas; Amegadzie, Albert; Kunz, Roxanne; Qian, Wenyuan; Chen, Ning; Tegley, Christopher M.; Demorin, Frenel; Yuan, Chester Chenguang; Liu, Qingyian; Zhu, Jiawang; Peterkin, Tanya; Adams, Jeffrey A.; Hu, Essa; Chavez, Frank, Jr.
PATENT ASSIGNEE(S): Amgen Inc., USA
SOURCE: PCT Int. Appl., 148pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2009075874	A1	20090618	WO 2008-US13639	20081212

W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

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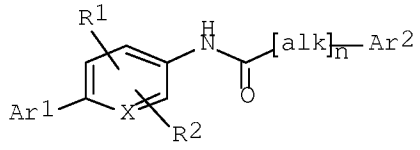
PRIORITY APPLN. INFO.: US 2007-7486P P 20071213

OTHER SOURCE(S): MARPAT 151:77918

GI



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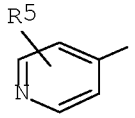
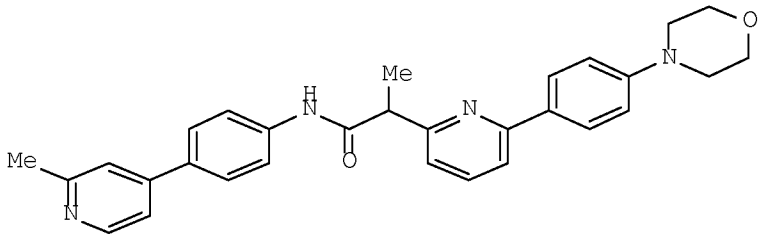


II



III

AB The title compds. I [n = 0-1; alk = alkylene optionally substituted with cycloalkyl or 1-3 F atoms; X = CH or N; R1, R2 = H, alkyl, alkoxy, etc.; Ar1 = II (wherein R5 = alkyl); Ar2 = (un)substituted aryl, heteroaryl, cycloalkyl, etc.; with the provisos] that are .gamma.-secretase modulators and are therefore useful for the treatment of diseases treatable by modulation of .gamma.-secretase such as Alzheimer's disease, were prepd. and formulated. E.g., a multi-step synthesis of III, starting from propiononitrile and 2,6-dichloropyridine, was given. Exemplified compds. I were tested for modulation of A.beta.-42 from HEK 293 cells over-expressing APP (data given for representative compds. I). Also provided are pharmaceutical compns. contg. compds. I and processes for prepg. such compds.

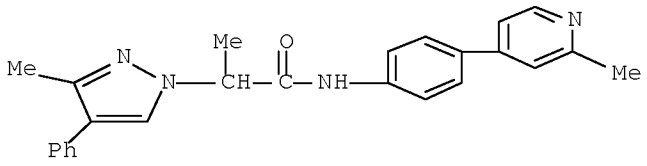
IT 1161359-59-6P 1161359-60-9P 1161359-85-8P 1161359-86-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of N-[4-(pyridin-4-yl)phenyl] amides as .gamma.-secretase modulators)

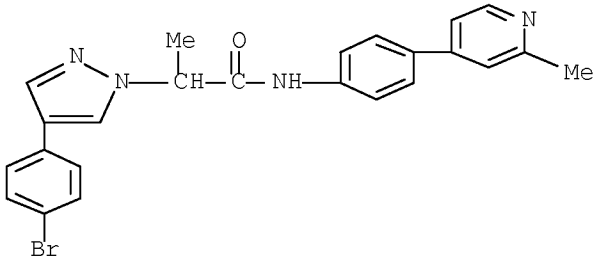
RN 1161359-59-6 CAPLUS

CN 1H-Pyrazole-1-acetamide, .alpha.,3-dimethyl-N-[4-(2-methyl-4-pyridinyl)phenyl]-4-phenyl- (CA INDEX NAME)



RN 1161359-60-9 CAPLUS

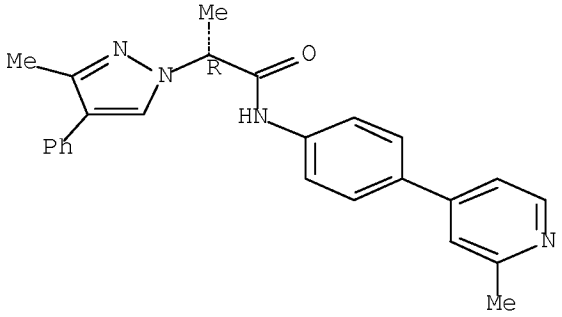
CN 1H-Pyrazole-1-acetamide, 4-(4-bromophenyl)-.alpha.-methyl-N-[4-(2-methyl-4-pyridinyl)phenyl]- (CA INDEX NAME)



RN 1161359-85-8 CAPLUS

CN 1H-Pyrazole-1-acetamide, .alpha.,3-dimethyl-N-[4-(2-methyl-4-pyridinyl)phenyl]-4-phenyl-, (.alpha.R)- (CA INDEX NAME)

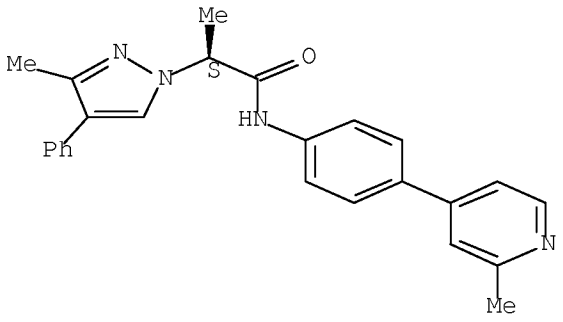
Absolute stereochemistry.



RN 1161359-86-9 CAPLUS

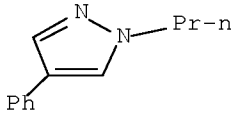
CN 1H-Pyrazole-1-acetamide, .alpha.,3-dimethyl-N-[4-(2-methyl-4-pyridinyl)phenyl]-4-phenyl-, (.alpha.S)- (CA INDEX NAME)

Absolute stereochemistry.

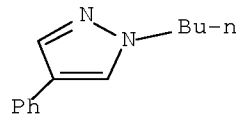


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

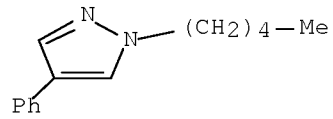
L14 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:813550 CAPLUS Full-text
DOCUMENT NUMBER: 149:332151
TITLE: Bu3SnH-Mediated radical cyclization onto azoles
AUTHOR(S): Allin, Steven M.; Barton, William R. S.; Russell Bowman, W.; Bridge, Emma; Elsegood, Mark R. J.; McInally, Tom; McKee, Vickie
CORPORATE SOURCE: Department of Chemistry, Loughborough University, Loughborough, Leicestershire, LE11 3TU, UK
SOURCE: Tetrahedron (2008), 64(33), 7745-7758
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:332151
AB Alkyl radicals have been cyclized onto pyrroles, imidazoles and pyrazoles, and acyl radicals cyclized onto pyrroles, using Bu3SnH-, (Me3Si)3SiH- and Bu3GeH-mediated arom. homolytic substitution for the synthesis of bicyclic N-heterocycles. The reactions yield intermediate .pi.-radicals that lose hydrogen in the rearomatization step of the arom. homolytic substitution. Mechanistic studies of these rearomatization steps indicate arom. homolytic substitution in which the initiator or breakdown products from the inhibitor are responsible for the H-abstraction step.
IT 457925-23-4P 457925-35-8P 457925-36-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Bu3SnH-mediated radical cyclization onto azoles)
RN 457925-23-4 CAPLUS
CN 1H-Pyrazole, 4-phenyl-1-propyl- (CA INDEX NAME)



RN 457925-35-8 CAPLUS
CN 1H-Pyrazole, 1-butyl-4-phenyl- (CA INDEX NAME)



RN 457925-36-9 CAPLUS
CN 1H-Pyrazole, 1-pentyl-4-phenyl- (CA INDEX NAME)



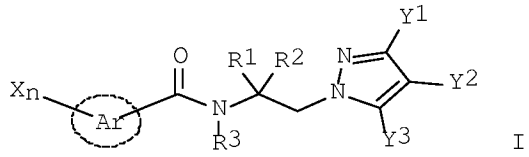
OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
REFERENCE COUNT: 80 THERE ARE 80 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:636634 CAPLUS Full-text
DOCUMENT NUMBER: 149:10000
TITLE: Preparation of novel pyrazole derivatives as harmful organism control agents, and use of the control agents
INVENTOR(S): Tanaka, Koji; Hasebe, Motohiro; Kuroki, Nobutaka; Suwa, Akiyuki
PATENT ASSIGNEE(S): Nihon Nohyaku Co., Ltd., Japan
SOURCE: PCT Int. Appl., 138pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

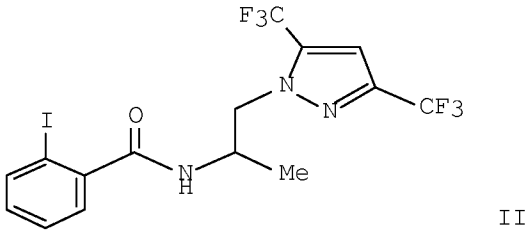
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008062878	A1	20080529	WO 2007-JP72682	20071122

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,

BY, KG, KZ, MD, RU, TJ, TM
PRIORITY APPLN. INFO.: JP 2006-316296 A 20061122
OTHER SOURCE(S): MARPAT 149:10000
GI



I



II

AB N-2-(substituted pyrazolyl)ethylcarboxamide derivs. represented by the general formula (I) or salts thereof [R1, R2 = H, C1-6 alkyl; or R1 and R2 together form C3-6 cycloalkane; R3 = H, C1-6 alkyl, C1-6 alkoxy-C1-6 alkyl, C1-6 alkylcarbonyl, C1-6 alkoxycarbonyl; Ar = Ph, pyridyl, pyrimidinyl, pyrazinyl, pyrazolyl, furyl, thienyl, oxazolyl, isoxazolyl, thiazolyl, isothiazolyl, thiadiazolyl; X = halo, cyano, NO2, C1-6 alkyl, halo-C1-6 alkyl, C3-6 cycloalkyl, C1-6 alkoxy, halo-C1-6 alkoxy, C1-6 alkylthio, halo-C1-6 alkylthio, C1-6 alkoxy-C1-6 alkylthio, C1-6 alkylsulfinyl, halo-C1-6 alkylsulfinyl, C1-6 alkylsulfonyl, halo-C1-6 alkylsulfonyl, NH2, mono- or di(C1-6 alkyl)amino, each ring-(un)substituted piperidino, Ph, PhO, phenyl-C1-6 alkyl, C1-6 alkoxyimino-C1-6 alkyl; n = an integer of 0-5; Y1, Y2, Y3 = H, halo, cyano, C1-6 alkyl, halo-C1-6 alkyl, C1-6 alkylcarbonyl, C1-6 alkoxy, halo-C1-6 alkoxy, C1-6 alkoxy-C1-6 alkyl, C1-6 alkylthio, halo-C1-6 alkylthio, C1-6 alkylsulfinyl, halo-C1-6 alkylsulfinyl, C1-6 alkylsulfonyl, halo-C1-6 alkylsulfonyl, NH2, mono- or di(C1-6 alkyl)amino, CONH2, mono- or di(C1-6 alkyl)carbamoyl, each (un)substituted Ph, heterocyclyl, or heterocyclylcarbonyl, etc.; or adjacent two Xs, Y1 and Y2, or Y2 and Y3 represent C3-5 alkylene, C3-5 alkenylene, C1-3 alkylenedioxy, or halo-C1-3 alkylenedioxy] were prepd. There is also disclosed a harmful organism control agent comprising the deriv. or the salt thereof as an active ingredient. These compds. exhibit controlling effect on plant pests with a wide spectrum of fungicidal or nematocidal activity. Thus, 0.26 g 2-[3,5-bis(trifluoromethyl)pyrazol-1-yl]-1- methylethylamine was mixed with 10 mL THF, followed by adding sequentially Et3N 0.30, 2-iodobenzoic acid 0.25, and 2-chloro-1-methylpyridinium iodide 0.31 g, and the resulting mixt. was stirred for 2 h to give 79% N-[2-[3,5-bis(trifluoromethyl)pyrazol-1-yl]-1-methylethyl]-2-iodobenzamide (II). II at 200 ppm controlled .gtoreq.70-79% Alternaria brassicae on cabbage leaves and Blumeria graminis hordei on barley seedlings.

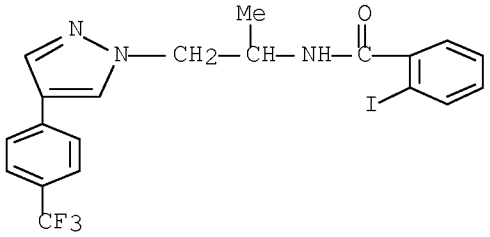
IT 1029143-96-1P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(prepn. of N-2-(substituted pyrazolyl)ethylcarboxamide derivs. as harmful organism control agents, in particular fungicides and nematocides)

RN 1029143-96-1 CAPLUS

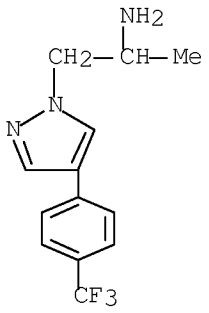
CN Benzamide, 2-iodo-N-[1-methyl-2-[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]ethyl]- (CA INDEX NAME)



IT 1029145-42-3P 1029145-65-0P 1029145-71-8P
1029414-81-0P 1029414-90-1P 1029414-96-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of N-2-(substituted pyrazolyl)ethylcarboxamide derivs. as harmful organism control agents, in particular fungicides and nematocides)

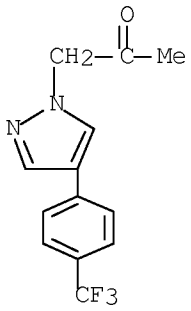
RN 1029145-42-3 CAPLUS

CN 1H-Pyrazole-1-ethanamine, .alpha.-methyl-4-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)

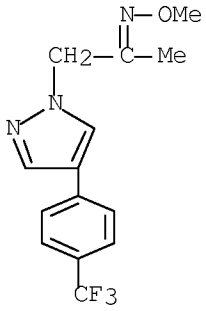


RN 1029145-65-0 CAPLUS

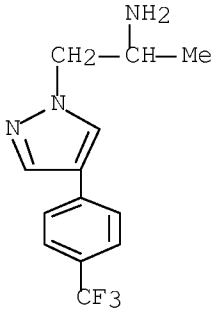
CN 2-Propanone, 1-[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]- (CA INDEX NAME)

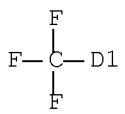


RN 1029145-71-8 CAPLUS
CN 2-Propanone, 1-[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]-, O-methyloxime (CA INDEX NAME)



RN 1029414-81-0 CAPLUS
CN 1H-Pyrazole-1-ethanamine, .alpha.,3(or .alpha.,5)-dimethyl-5(or 3)-(trifluoromethyl)-4-[4-(trifluoromethyl)phenyl]-, (.alpha.S)- (CA INDEX NAME)



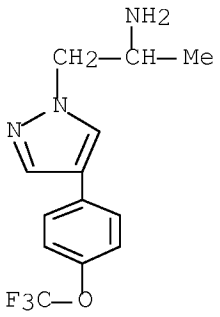


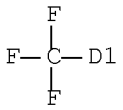
PAGE 2-A

D1—Me

RN 1029414-90-1 CAPLUS
CN 1H-Pyrazole-1-ethanamine, .alpha.,3(or .alpha.,5)-dimethyl-5(or 3)-(trifluoromethyl)-4-[4-(trifluoromethoxy)phenyl]-, (.alpha.S)- (CA INDEX NAME)

PAGE 1-A

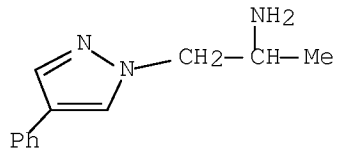




PAGE 2-A

D1—Me

RN 1029414-96-7 CAPLUS
CN 1H-Pyrazole-1-ethanamine, 3(or 5)-chloro-.alpha.-methyl-5(or 3)-(methylthio)-4-phenyl-, (.alpha.S)- (CA INDEX NAME)



D1—S—Me

D1—Cl

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:509883 CAPLUS Full-text
DOCUMENT NUMBER: 146:501057
TITLE: Antifungal triazole derivatives, processes for preparing them, and pharmaceutical compositions containing them
INVENTOR(S): Park, Joon Seok; Yu, Kyung A.; Kim, Sun Young; Song, Yeon Jung; Kim, Kang-Pil; Yoon, Yun Soo; Han, Mi Ryeong
PATENT ASSIGNEE(S): Daewoong Pharmaceutical Co., Ltd., S. Korea
SOURCE: PCT Int. Appl., 62pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007052943	A1	20070510	WO 2006-KR4495	20061031
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 1951705	A1	20080806	EP 2006-812334	20061031
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
JP 2009513698	T	20090402	JP 2008-538814	20061031
US 20080287440	A1	20081120	US 2008-92156	20080430
IN 2008DN04370	A	20080815	IN 2008-DN4370	20080522
KR 2008088583	A	20081002	KR 2008-712856	20080528
CN 101365692	A	20090211	CN 2006-80049309	20080626

PRIORITY APPLN. INFO.: KR 2005-103142 A 20051031
WO 2006-KR4495 W 20061031

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
GI

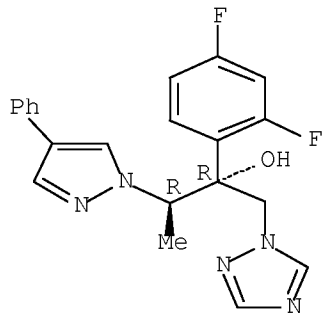
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to antifungal triazole derivs. I, processes for prepg. them, and pharmaceutical prepns. comprising them. In compd. I, Ar is C6-20 aryl substituted with .gtoreq. 1 halo or CF3; R1 is H, F, or C1-4 alkyl; R2, R3, and R4 independently represent H, halo, NO2, CN, NH2, OH, (cyclo|halo)alkyl, alkoxy, (un)substituted (hetero)aryl; including pharmaceutically acceptable salts thereof. For instance, the invention compd. II was prepd. by protection of 4-bromo-1H-pyrazole with trityl chloride followed by cross-coupling with 4-fluorophenylboronic acid (51%), deprotection (81%), and addn. to compd. III (56%). The antifungal activities of I were tested, e.g., the invention compd. IV had MIC values of .ltoreq. 0.015 .mu.g/mL against Candida albicans, 0.25 .mu.g/mL against Candida krusei, etc.

IT 936357-13-0P 936357-28-7P 936357-29-8P
936357-30-1P 936357-34-5P 936357-36-7P
936357-45-8P 936357-47-0P 936357-53-8P
936357-54-9P 936358-20-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; prepn. of antifungal triazole derivs.)

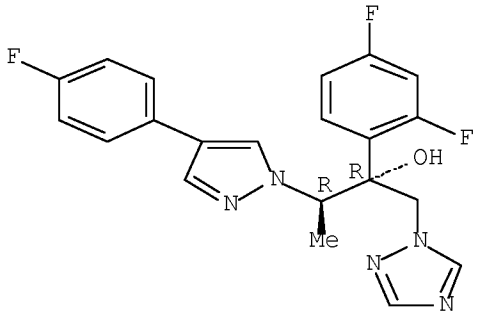
RN 936357-13-0 CAPLUS
CN 1H-1,2,4-Triazole-1-ethanol, .alpha.-(2,4-difluorophenyl)-.alpha.-[(1R)-1-(4-phenyl-1H-pyrazol-1-yl)ethyl]-, (.alpha.R)- (CA INDEX NAME)

Absolute stereochemistry.



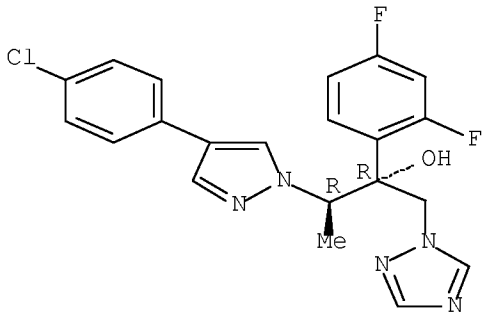
RN 936357-28-7 CAPLUS
CN 1H-1,2,4-Triazole-1-ethanol, .alpha.-(2,4-difluorophenyl)-.alpha.-[(1R)-1-[4-(4-fluorophenyl)-1H-pyrazol-1-yl]ethyl]-, (.alpha.R)- (CA INDEX NAME)

Absolute stereochemistry.



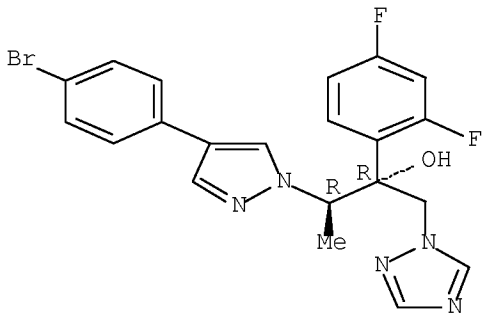
RN 936357-29-8 CAPLUS
CN 1H-1,2,4-Triazole-1-ethanol, .alpha.-[(1R)-1-[4-(4-chlorophenyl)-1H-pyrazol-1-yl]ethyl]-.alpha.-(2,4-difluorophenyl)-, (.alpha.R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 936357-30-1 CAPLUS
CN 1H-1,2,4-Triazole-1-ethanol, .alpha.-[(1R)-1-[4-(4-bromophenyl)-1H-pyrazol-1-yl]ethyl]-.alpha.-(2,4-difluorophenyl)-, (.alpha.R)- (CA INDEX NAME)

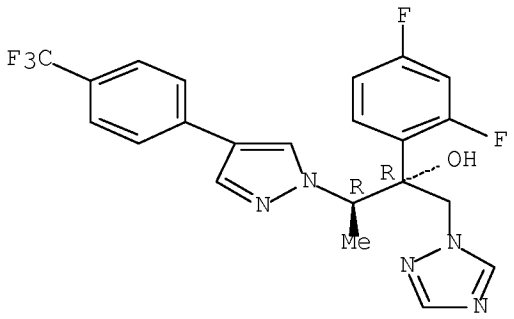
Absolute stereochemistry.



RN 936357-34-5 CAPLUS
CN 1H-1,2,4-Triazole-1-ethanol, .alpha.-(2,4-difluorophenyl)-.alpha.-[(1R)-1-[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]ethyl]-, (.alpha.R)- (CA

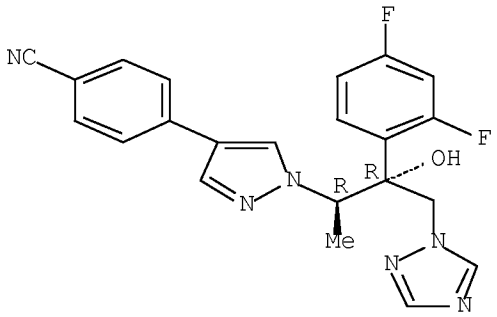
INDEX NAME)

Absolute stereochemistry.



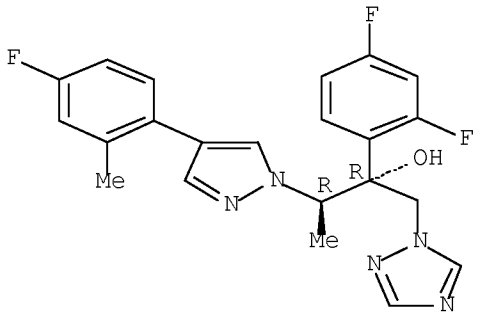
RN 936357-36-7 CAPLUS
CN Benzonitrile, 4-[1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-1H-pyrazol-4-yl]- (CA INDEX NAME)

Absolute stereochemistry.



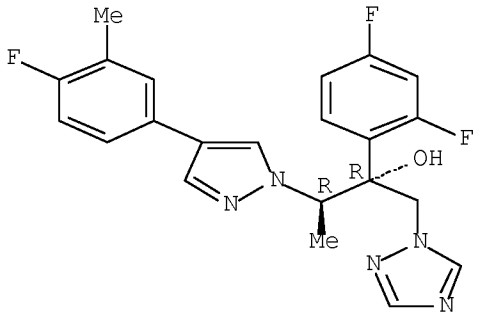
RN 936357-45-8 CAPLUS
CN 1H-1,2,4-Triazole-1-ethanol, .alpha.-(2,4-difluorophenyl)-.alpha.-[(1R)-1-[4-(4-fluoro-2-methylphenyl)-1H-pyrazol-1-yl]ethyl]-, (.alpha.R)- (CA INDEX NAME)

Absolute stereochemistry.



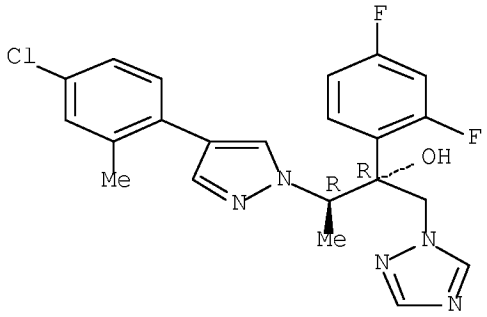
RN 936357-47-0 CAPLUS
CN 1H-1,2,4-Triazole-1-ethanol, .alpha.-(2,4-difluorophenyl)-.alpha.-[(1R)-1-[4-(4-fluoro-3-methylphenyl)-1H-pyrazol-1-yl]ethyl]-, (.alpha.R)- (CA INDEX NAME)

Absolute stereochemistry.



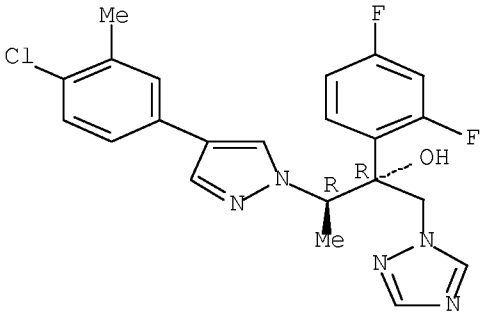
RN 936357-53-8 CAPLUS
CN 1H-1,2,4-Triazole-1-ethanol, .alpha.-[(1R)-1-[4-(4-chloro-2-methylphenyl)-1H-pyrazol-1-yl]ethyl]-.alpha.-(2,4-difluorophenyl)-, (.alpha.R)- (CA INDEX NAME)

Absolute stereochemistry.



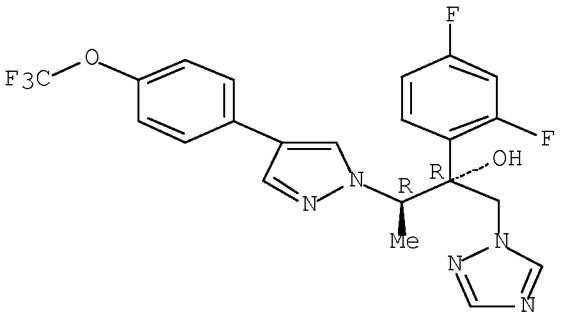
RN 936357-54-9 CAPLUS
CN 1H-1,2,4-Triazole-1-ethanol, .alpha.-[(1R)-1-[4-(4-chloro-3-methylphenyl)-1H-pyrazol-1-yl]ethyl]-.alpha.-(2,4-difluorophenyl)-, (.alpha.R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 936358-20-2 CAPLUS
CN 1H-1,2,4-Triazole-1-ethanol, .alpha.-(2,4-difluorophenyl)-.alpha.-[(1R)-1-[4-[4-(trifluoromethoxy)phenyl]-1H-pyrazol-1-yl]ethyl]-, (.alpha.R)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:2709 CAPLUS Full-text
DOCUMENT NUMBER: 146:176187
TITLE: Acyclic, orally bioavailable ketone-based cathepsin K inhibitors
AUTHOR(S): Barrett, David G.; Catalano, John G.; Deaton, David N.; Long, Stacey T.; McFadyen, Robert B.; Miller, Aaron B.; Miller, Larry R.; Samano, Vicente; Tavares, Francis X.; Wells-Knecht, Kevin J.; Wright, Lois L.; Zhou, Hui-Qiang Q.
CORPORATE SOURCE: Department of Medicinal Chemistry, GlaxoSmithKline, Research Triangle Park, NC, 27709, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2007), 17(1), 22-27
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:176187
AB Starting from a potent ketone-based inhibitor with poor drug properties, incorporation of P2-P3 elements from a ketoamide-based inhibitor led to the

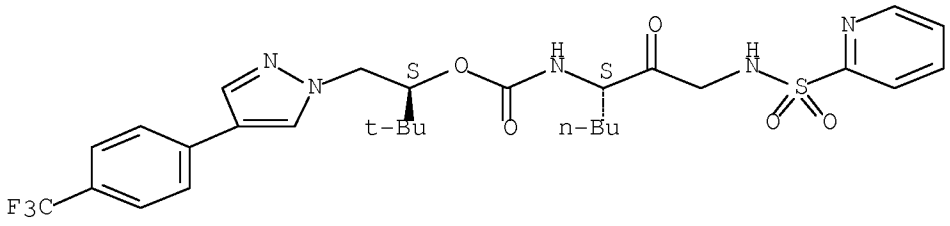
identification of a hybrid series of ketone-based cathepsin K inhibitors with better oral bioavailability than the starting ketone.

IT 511268-49-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(acyclic, orally bioavailable ketone-based cathepsin K inhibitors)

RN 511268-49-8 CAPLUS

CN Carbamic acid, N-[(1S)-1-[2-[(2-pyridinylsulfonyl)amino]acetyl]pentyl]-, (1S)-2,2-dimethyl-1-[[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]methyl]propyl ester (CA INDEX NAME)

Absolute stereochemistry.

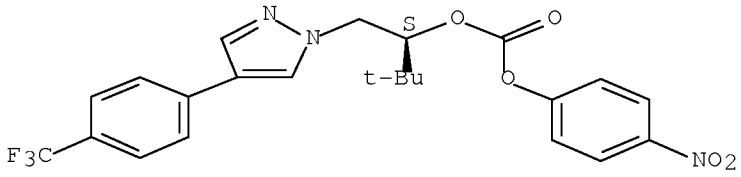


IT 497947-00-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(acyclic, orally bioavailable ketone-based cathepsin K inhibitors)

RN 497947-00-9 CAPLUS

CN Carbonic acid, (1S)-2,2-dimethyl-1-[[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]methyl]propyl 4-nitrophenyl ester (CA INDEX NAME)

Absolute stereochemistry.

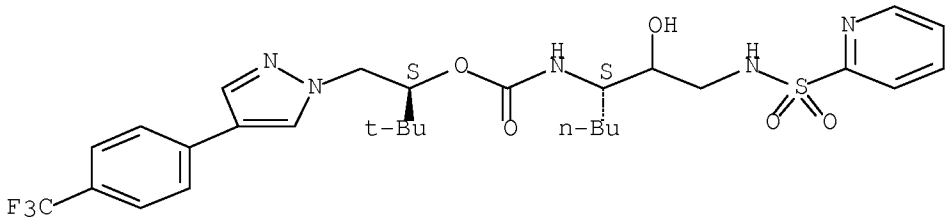


IT 921206-74-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(acyclic, orally bioavailable ketone-based cathepsin K inhibitors)

RN 921206-74-8 CAPLUS

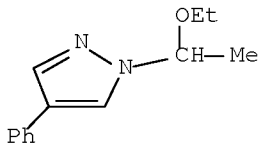
CN Carbamic acid, N-[(1S)-1-[1-hydroxy-2-[(2-pyridinylsulfonyl)amino]ethyl]pentyl]-, (1S)-2,2-dimethyl-1-[[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]methyl]propyl ester (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:636024 CAPLUS Full-text
DOCUMENT NUMBER: 143:266862
TITLE: Pd-EDTA as an efficient catalyst for Suzuki-Miyaura reactions in water
AUTHOR(S): Korolev, Dmitrii N.; Bumagin, Nikolay A.
CORPORATE SOURCE: Department of Chemistry, Lomonosov MSU, Moscow, 119992, Russia
SOURCE: Tetrahedron Letters (2005), 46(34), 5751-5754
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:266862
AB PdCl2-EDTA complex is an efficient catalyst for the Suzuki-Miyaura reactions of aryl and heteroaryl halides with aryl(heteroaryl)boronic acids in water at 20-100 .degree.C. Aryl iodides and bromides undergo the cross-coupling with turnover nos. (TON) up to 97,000 and turnover frequencies up to 582,000 h-1.
IT 863921-50-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Suzuki-Miyaura reaction of aryl and heteroaryl halides with aryl(heteroaryl)boronic acids in water using palladium-EDTA catalyst)
RN 863921-50-0 CAPLUS
CN 1H-Pyrazole, 1-(1-ethoxyethyl)-4-phenyl- (CA INDEX NAME)

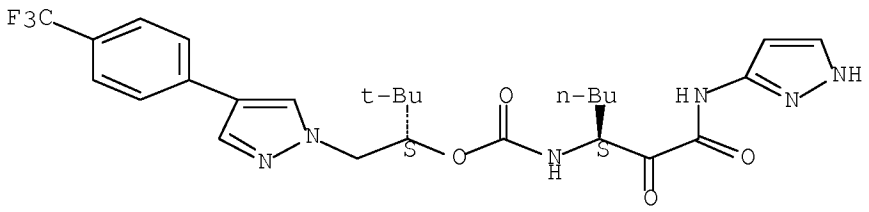


OS.CITING REF COUNT: 26 THERE ARE 26 CAPLUS RECORDS THAT CITE THIS RECORD (26 CITINGS)
REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:589354 CAPLUS Full-text

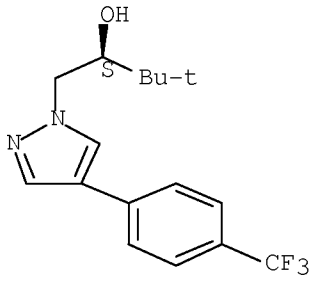
DOCUMENT NUMBER: 143:259481
TITLE: P2-P3 conformationally constrained ketoamide-based inhibitors of cathepsin K
AUTHOR(S): Barrett, David G.; Boncek, Virginia M.; Catalano, John G.; Deaton, David N.; Hassell, Anne M.; Jurgensen, Cynthia H.; Long, Stacey T.; McFadyen, Robert B.; Miller, Aaron B.; Miller, Larry R.; Payne, J. Alan; Ray, John A.; Samano, Vicente; Shewchuk, Lisa M.; Tavares, Francis X.; Wells-Knecht, Kevin J.; Willard, Derril H.; Wright, Lois L.; Zhou, Hui-Qiang Q.
CORPORATE SOURCE: Department of Medicinal Chemistry, GlaxoSmithKline, Research Triangle Park, NC, 27709, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(15), 3540-3546
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:259481
AB An orally bioavailable series of ketoamide-based cathepsin K inhibitors with good pharmacokinetic properties has been identified. Starting from a potent inhibitor endowed with poor drug properties, conformational constraint of the P2-P3 linker and modifications to P 1 ' elements led to an enhancement in potency, soly., clearance, and bioavailability. These optimized inhibitors attenuated bone resorption in a rat TPTX hypocalcemic bone resorption model.
IT 497946-97-1P
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(P2-P3 conformationally constrained ketoamide-based inhibitors of cathepsin K)
RN 497946-97-1 CAPLUS
CN Carbamic acid, [(1S)-1-[oxo(1H-pyrazol-3-ylamino)acetyl]pentyl]-, (1S)-2,2-dimethyl-1-[[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]methyl]propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



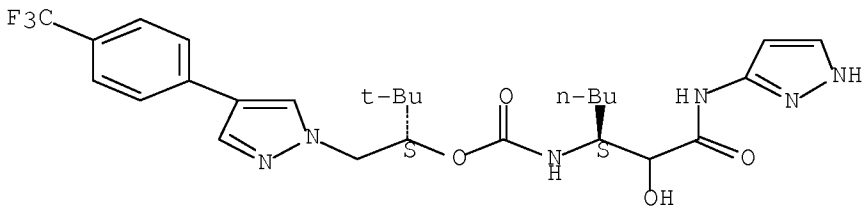
IT 497946-99-3P 879224-70-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(P2-P3 conformationally constrained ketoamide-based inhibitors of cathepsin K)
RN 497946-99-3 CAPLUS
CN 1H-Pyrazole-1-ethanol, .alpha.-(1,1-dimethylethyl)-4-[4-(trifluoromethyl)phenyl]-, (.alpha.S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 879224-70-1 CAPLUS
CN Carbamic acid, [(1S)-1-[1-hydroxy-2-oxo-2-(1H-pyrazol-3-ylamino)ethyl]pentyl]-, (1S)-2,2-dimethyl-1-[[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]methyl]propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 14 THERE ARE 14 CAPLUS RECORDS THAT CITE THIS RECORD (14 CITINGS)
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:872790 CAPLUS Full-text
DOCUMENT NUMBER: 141:350155
TITLE: Preparation of phenyl-substituted heterocycles as MIF inhibitors for the treatment of inflammatory diseases
INVENTOR(S): Morand, Eric Francis; Iskander, Magdy Naguib; Skene, Colin Edward
PATENT ASSIGNEE(S): Cortical Pty. Ltd., Australia
SOURCE: PCT Int. Appl., 144 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004089927	A1	20041021	WO 2004-AU453	20040407

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,

LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
TD, TG

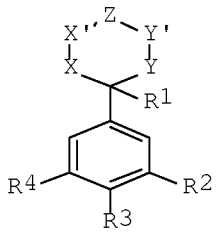
				Current application
AU 2004228069	A1	20041021	AU 2004-228069	20040407
CA 2521606	A1	20041021	CA 2004-2521606	20040407
EP 1611120	A1	20060104	EP 2004-726068	20040407
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
JP 2006522025	T	20060928	JP 2006-504000	20040407
US 20070010563	A1	20070111	US 2005-552595	20051007
IN 2005KN02068	A	20060922	IN 2005-KN2068	20051021
ZA 2005008847	A	20061025	ZA 2005-8847	20051101
IN 2008KN02178	A	20090116	IN 2008-KN2178	20080530

PRIORITY APPLN. INFO.:

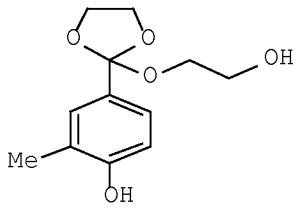
AU 2003-901579	A	20030407
AU 2003-906773	A	20031208
WO 2004-AU453	W	20040407
IN 2005-KN2068	A3	20051021

OTHER SOURCE(S): MARPAT 141:350155

GI



I



II

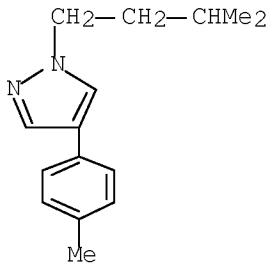
AB Title compds. I [wherein X, X', Y, Y' = independently C(R5)2, O, S, NR5; Z = a bond, C(R5)2, O, S, NR5; or XX', YY', X'Z, or Y'Z = CR5=CR5, CR5=N, N=CR5, N=N; R1 = H, alkyl, alkenyl, alkynyl, acyl, alkoxy, alkylthio, amino, etc.; R2, R4 = independently H, alkyl, hydroxy(alkyl), mercapto(alkyl), haloalkyl, nitroalkyl, etc.; R3 = alkyl, hydroxy(alkyl), mercapto(alkyl), haloalkyl, nitroalkyl, (hetero)aryl(alkyl), etc.; with provisos; or pharmaceutically acceptable salts or prodrugs thereof] were prepd. for inhibiting the cytokine or biol. activity of macrophage migration inhibitory factor (MIF). Examples include syntheses for forty-five invention compds. and eight bioassays. For instance, reaction of 3-methyl-4-hydroxybenzaldehyde with ethylene glycol in the presence of p-toluenesulfonic acid in toluene provided the dioxolane II (24%). The latter significantly inhibited the induction of S112 human fibroblast proliferation at 1 nM and suppressed MIF-dependent IL-1 induced fibroblast cyclooxygenase-2 expression by 10.5% at 0.01 .mu.M up to 31.4% at 50 .mu.M. No cytotoxicity, i.e., no significant increase in apoptotic cells or decrease in viable cells, resulted from treatment of S112 human dermal fibroblasts with therapeutic concns. (50 .mu.M) of II. Thus, I and their pharmaceutical compns. are useful for treating autoimmune diseases, tumors, or inflammatory diseases.

IT 777063-42-0P, 1-(3-Methylbutyl)-4-(4-methylphenyl)-1H-pyrazole

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(MIF inhibitor; prepn. of Ph-substituted heterocycles as MIF inhibitors for treatment of inflammatory diseases, tumors, or autoimmune diseases)

RN 777063-42-0 CAPLUS

CN 1H-Pyrazole, 1-(3-methylbutyl)-4-(4-methylphenyl)- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:231322 CAPLUS Full-text

DOCUMENT NUMBER: 140:390938

TITLE: Tributylgermanium hydride as a replacement for tributyltin hydride in radical reactions

AUTHOR(S): Bowman, W. Russell; Krintel, Sussie L.; Schilling, Mark B.

CORPORATE SOURCE: Department of Chemistry, Loughborough University, Loughborough, LE1 3TU, UK

SOURCE: Organic & Biomolecular Chemistry (2004), 2(4), 585-592
CODEN: OBCRAK; ISSN: 1477-0520

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

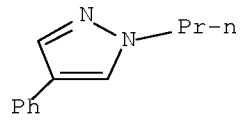
OTHER SOURCE(S): CASREACT 140:390938

AB Tributylgermanium hydride (Bu3GeH) can be used as an alternative to tributyltin hydride (Bu3SnH) as a radical generating reagent with a wide range of radical substrates. Tributylgermanium hydride has several practical advantages over tributyltin hydride, e.g. low toxicity, good stability and much easier work-up of reactions. The reagent can be easily prepd. in good yield and stored indefinitely. Suitable substrates include iodides, bromides, activated chlorides, Ph selenides, tert-nitroalkanes, thiocarbonylimidazolides and Barton esters. Alkyl, vinyl and aryl radicals can be generated in radical reactions including redn. and cyclization processes. Common radical initiators such as ACCN and triethylborane can be used. The slower rate of hydrogen abstraction by carbon-centered radicals from Bu3GeH as compared to Bu3SnH facilitates improved cyclisation yields. Polarity reversal catalysis (PRC) with phenylthiol can be used in reactions which generate stable radical intermediates which will not abstr. hydrogen from Bu3GeH.

IT 457925-23-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(tributylgermanium hydride as a replacement for tributyltin hydride in

radical reactions)
RN 457925-23-4 CAPLUS
CN 1H-Pyrazole, 4-phenyl-1-propyl- (CA INDEX NAME)

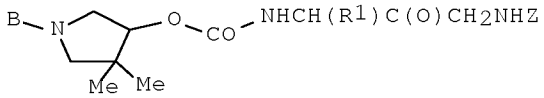


OS.CITING REF COUNT: 28 THERE ARE 28 CAPLUS RECORDS THAT CITE THIS RECORD (28 CITINGS)
REFERENCE COUNT: 80 THERE ARE 80 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:301078 CAPLUS Full-text
DOCUMENT NUMBER: 138:304173
TITLE: Preparation of pyridinylsulfonylamino-contg. keto carbamates as inhibitors of cathepsin K useful against osteoporosis and other disorders
INVENTOR(S): Deaton, David Norman; Catalano, John George
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 119 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003031437	A1	20030417	WO 2002-US31480	20021002
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002334808	A1	20030422	AU 2002-334808	20021002
EP 1448554	A1	20040825	EP 2002-800886	20021002
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2005537216	T	20051208	JP 2003-534420	20021002
US 20050043368	A1	20050224	US 2004-492059	20040408
US 7288541	B2	20071030		

PRIORITY APPLN. INFO.: US 2001-327938P P 20011009
WO 2002-US31480 W 20021002
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 138:304173
GI



I

AB The present invention includes pyridinylsulfonylamino-contg. keto carbamates (ACH(R1)DC(O)NHCH(R2)C(O)CH2NHZ (I) and II; variables defined below; e.g. (1S)-2,2-dimethyl-1-[[3-[4-(trifluoromethyl)phenyl]-1H-pyrazol- 1-yl]methyl]propyl 2-oxo-3-[(2-pyridinylsulfonyl)amino]propylcarbamate), which are useful as cathepsin K inhibitors. The described invention also includes methods of making such ketone derivs. as well as methods of using the same in the treatment of disorders, including osteoporosis. Although the methods of prepn. are not claimed, 19 example prepns. are included. Each of the compds. exemplified in the Examples section bind with high affinity (IC50 < 10 .mu.M) to the cathepsin K enzyme, e.g. (1S)-1-[[4-(1H-imidazol-1-yl)phenoxy]methyl]-2,2-dimethylpropyl (1S)-1-[[(2-pyridinylsulfonyl)amino]acetyl]pentylcarbamate exhibits an IC50 of .apprx.10-1 nM or less. For I: A = (Q3)p-(Q2)n -(Q1)-(Q)m- (Q is CH2 and m = 0-2, or Q is OCH2 and m is 1, or Q is N(R3)CH2 and m is 1, where R3 is H or C1-C6 alkyl; Q1 is aryl, heteroaryl, or heterocyclyl; Q2 is CH2 and n is 0 or 1, or Q2 is O and n is 1, or Q2 is N(R3) and n is 1, where R3 is H or C1-C6 alkyl; Q3 is aryl or heteroaryl and p is 0 or 1). R1 is alkyl or cycloalkyl, said cycloalkyl may be optionally substituted with alkyl; D is O or S; R2 is H or alkyl; and Z is -(X1)q-(X2) (X1 is S(O)2, C(O), or -CH2-, and q = 0-2; and X2 is aryl, heteroaryl, or heterocyclyl). For II: B is -(Q1)a-(Q2)b-(Q3) (Q1 is C(O), S(O)2, or CR2R3, where R2 and R3 each = H or C1-C6 alkyl, and a = 0-3; Q2 is O, S, NR2, or CR2R3, where R2 and R3 each = H or C1-C6 alkyl, and b = 0-3; and Q3 is aryl, heteroaryl, heterocyclyl, aralkyl, or alkyleneheterocyclyl). R1 is H or alkyl; Z is -(X1)q-(X2) (X1 is S(O)2, C(O), or alkyl, and q is 0 or 1; and X2 is aryl, heteroaryl, or heterocyclyl).

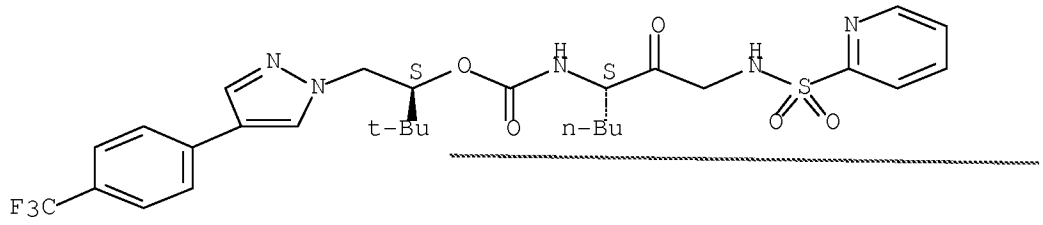
IT 511268-49-8P, (1S)-2,2-Dimethyl-1-[[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]methyl]propyl (1S)-1-[[(2-pyridinylsulfonyl)amino]acetyl]pentylcarbamate
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; prepn. of pyridinylsulfonylamino-contg. keto carbamates as inhibitors of cathepsin K useful against osteoporosis and other disorders)

RN 511268-49-8 CAPLUS

CN Carbamic acid, N-[(1S)-1-[2-[(2-pyridinylsulfonyl)amino]acetyl]pentyl]-, (1S)-2,2-dimethyl-1-[[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]methyl]propyl ester (CA INDEX NAME)

Absolute stereochemistry.

102a/102e---103a

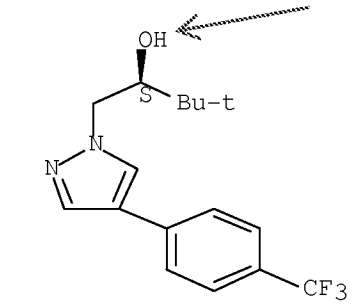


IT 497946-99-3P, (2S)-3,3-Dimethyl-1-[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]-2-butanol 497947-00-9P, (1S)-2,2-Dimethyl-1-[[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]methyl]propyl 4-nitrophenyl carbonate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of pyridinylsulfonylamino-contg. keto carbamates as inhibitors of cathepsin K useful against osteoporosis and other disorders)

RN 497946-99-3 CAPLUS

CN 1H-Pyrazole-1-ethanol, .alpha.-(1,1-dimethylethyl)-4-[4-(trifluoromethyl)phenyl]-, (.alpha.S)- (CA INDEX NAME)

Absolute stereochemistry.

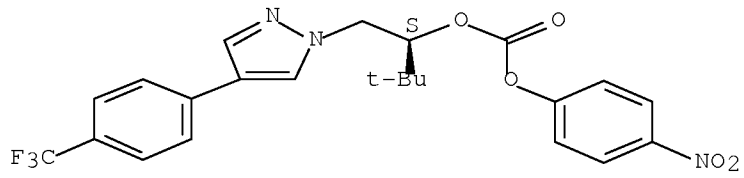


102a/102e

RN 497947-00-9 CAPLUS

CN Carbonic acid, (1S)-2,2-dimethyl-1-[[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]methyl]propyl 4-nitrophenyl ester (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:133034 CAPLUS Full-text
DOCUMENT NUMBER: 138:187774
TITLE: Preparation of .alpha.-ketoamide derivatives as cathepsin K inhibitors useful against bone disorders such as osteoporosis
INVENTOR(S): Barrett, David Gene; Deaton, David Norman; McFadyen, Robert Blount; Miller, Aaron Bayne; Ray, John Albert; Tavares, Francis Xavier; Zhou, Huiqiang
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA; Samano, Vicente
SOURCE: PCT Int. Appl., 261 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003013518	A1	20030220	WO 2002-US23255		20020723
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2002355394	A1	20030224	AU 2002-355394		20020723
EP 1411933	A1	20040428	EP 2002-752509		20020723
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK					
JP 2005504040	T	20050210	JP 2003-518527		20020723
US 20050107616	A1	20050519	US 2004-485656		20040721
PRIORITY APPLN. INFO.:			US 2001-310169P	P	20010803
			WO 2002-US23255	W	20020723

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 138:187774
AB Bi-aryl/heteroaryl ketoamide derivs. ACH(R1)DC(O)NHCH(CH2CH2CH2CH2R2)C(O)C(O)NHZ (I; variables defined below; e.g. (1S)-2,2-dimethyl-1-[[3-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]methyl]propyl (1S)-1-[oxo[(1H-pyrazol-5-ylmethyl)amino]acetyl]pentylcarbamate), useful as cathepsin K inhibitors, are described herein. The described invention also includes methods of making such I as well as methods of using the same in the treatment of disorders, including osteoporosis, assocd. with enhanced bone turnover which can ultimately lead to fracture. For I: A = (Q3)p-(Q2)n -(Q1)-(Q)m-, wherein Q is CH2 and m is 0, 1, or 2, or Q is OCH2 and m is 1, or Q is N(R')CH2 and m is 1, where R' is H or C1-C6 alkyl; Q1 is aryl or heteroaryl; Q2 is CH2 and n is 0, or 1, or Q2 is CH2O and n is 1, or Q2 is N(R') and n is 1, where R' is H or C1-C6 alkyl; Q3 is aryl or heteroaryl and p is 0 or 1; R' is C1-C6 alkyl, C3-C6 cycloalkyl or C3-C6 cycloalkyl substituted with C1-C6 alkyl; D is O or S; R2 is H or -NR3R4; R3, R6, and R7 = H or C1-C6 alkyl; R4 is H, C1-C6 alkyl, -C(O)R5, -C(O)OR5, -S(O)2R5; R5 is H, C1-C6 alkyl, or -NR6R7; Z = -(X)m-(X1), wherein X is C(R'')(R'''), wherein R'' is H or C1-C6 alkyl, R''' is H or C1-C6 alkyl, and m is 0, 1, or 2; and X1 is aryl, heteroaryl, or heterocyclyl.

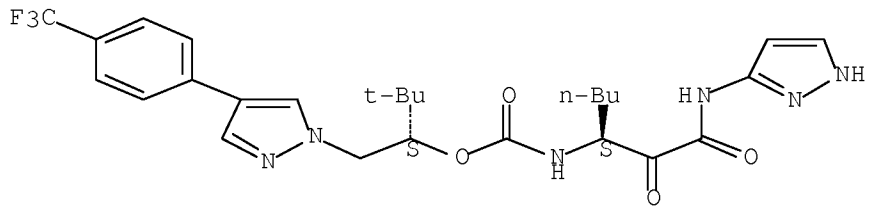
Although the methods of prepn. are not claimed, 65 example prepns. of I and intermediates are included. Each of I in the Examples section bind with high affinity (IC50 < 10 .mu.M) to the cathepsin K enzyme; for example, IC50 = 1-0.01 nM for (1S)-2,2-dimethyl-1-[[3-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]methyl]propyl (1S)-1-[oxo[(1H-pyrazol-5-ylmethyl)amino]acetyl]pentylcarbamate. Inhibition results for 7 examples of I are tabulated for different cathepsins (human and/or rat B, H, K, L, S, V).

IT 497946-97-1P, (1S)-2,2-Dimethyl-1-[[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]methyl]propyl [(1S)-1-[oxo(1H-pyrazol-3-ylamino)acetyl]pentyl]carbamate
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; prepn. of .alpha.-ketoamide derivs. as cathepsin K inhibitors useful against bone disorders such as osteoporosis)

RN 497946-97-1 CAPLUS

CN Carbamic acid, [(1S)-1-[oxo(1H-pyrazol-3-ylamino)acetyl]pentyl]-, (1S)-2,2-dimethyl-1-[[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]methyl]propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

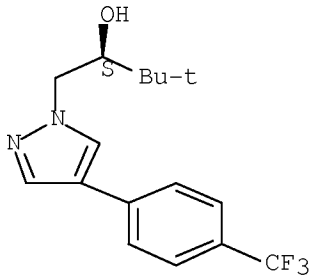


IT 497946-99-3P, (2S)-3,3-Dimethyl-1-[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]-2-butanol 497947-00-9P, (1S)-2,2-Dimethyl-1-[[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]methyl]propyl 4-nitrophenyl carbonate 497947-01-0P, (1S)-2,2-Dimethyl-1-[[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]methyl]propyl [(1S)-1-[(1R)-1-hydroxy-2-oxo-2-(1H-pyrazol-3-ylamino)ethyl]pentyl]carbamate 497947-02-1P, (1S)-2,2-Dimethyl-1-[[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]methyl]propyl [(1S)-1-[(1S)-1-hydroxy-2-oxo-2-(1H-pyrazol-3-ylamino)ethyl]pentyl]carbamate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of .alpha.-ketoamide derivs. as cathepsin K inhibitors useful against bone disorders such as osteoporosis)

RN 497946-99-3 CAPLUS

CN 1H-Pyrazole-1-ethanol, .alpha.-(1,1-dimethylethyl)-4-[4-(trifluoromethyl)phenyl]-, (.alpha.S)- (CA INDEX NAME)

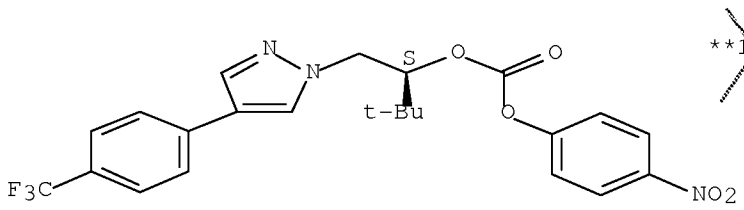
Absolute stereochemistry.



102b

RN 497947-00-9 CAPLUS
CN Carbonic acid, (1S)-2,2-dimethyl-1-[[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]methyl]propyl 4-nitrophenyl ester (CA INDEX NAME)

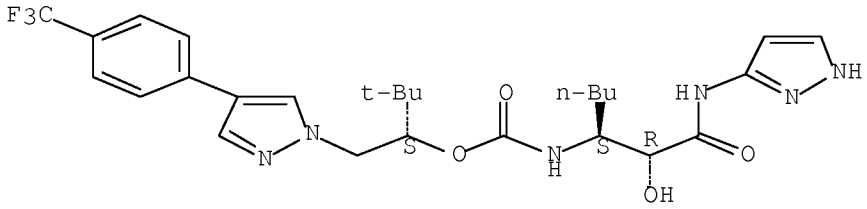
Absolute stereochemistry.



~~**102b/103a**~~

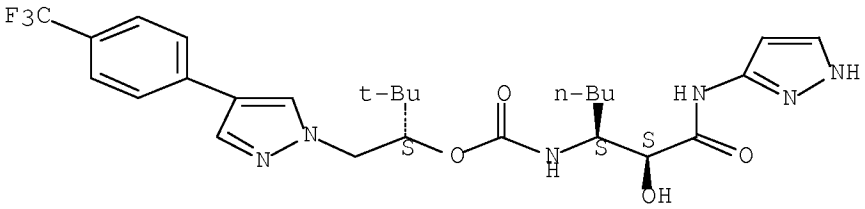
RN 497947-01-0 CAPLUS
CN Carbamic acid, [(1S)-1-[(1R)-1-hydroxy-2-oxo-2-(1H-pyrazol-3-ylamino)ethyl]pentyl]-, (1S)-2,2-dimethyl-1-[[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]methyl]propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 497947-02-1 CAPLUS
CN Carbamic acid, [(1S)-1-[(1S)-1-hydroxy-2-oxo-2-(1H-pyrazol-3-ylamino)ethyl]pentyl]-, (1S)-2,2-dimethyl-1-[[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]methyl]propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



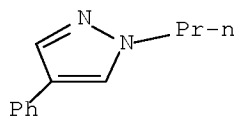
OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:379222 CAPLUS Full-text
DOCUMENT NUMBER: 137:232795
TITLE: Radical cyclisation onto pyrazoles: synthesis of withasomnine
AUTHOR(S): Allin, Steven M.; Barton, William R. S.; Bowman, W. Russell; McInally, Tom
CORPORATE SOURCE: Department of Chemistry, Loughborough University, Loughborough, LE11 3TU, UK
SOURCE: Tetrahedron Letters (2002), 43(23), 4191-4193
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:232795

AB A novel synthetic protocol for the synthesis of [1,2-b]-fused bicyclic pyrazoles has been developed using radical cyclization. The protocol uses cyclisation of pyrazole-1-(.omega.-alkyl) radicals generated from 1-[.omega.-(phenylselenyl)alkyl]-pyrazole precursors. The pyrazole natural product, withasomnine (3-phenyl-5,6-dihydro-4H-pyrrolo[1,2- b]pyrazole), and larger ring analogs have been synthesized in good yield using the protocol. A Bu3SnH-mediated oxidative cyclisation mechanism is facilitated by azo or Et3B radical initiators acting as oxidants of the intermediate .pi.-radicals.

IT 457925-23-4P 457925-35-8P 457925-36-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of withasomnine and other [1,2-b]-fused bicyclic pyrazoles via a radical cyclization onto pyrazoles)

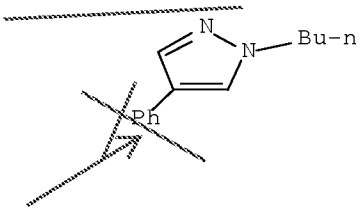
RN 457925-23-4 CAPLUS
CN 1H-Pyrazole, 4-phenyl-1-propyl- (CA INDEX NAME)



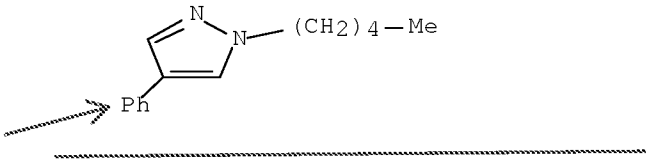
RN 457925-35-8 CAPLUS
CN 1H-Pyrazole, 1-butyl-4-phenyl- (CA INDEX NAME)

R3

H Vs -CH3

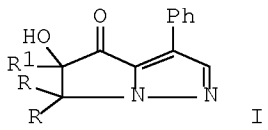


RN 457925-36-9 CAPLUS
CN 1H-Pyrazole, 1-pentyl-4-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 26 THERE ARE 26 CAPLUS RECORDS THAT CITE THIS RECORD (28 CITINGS)
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

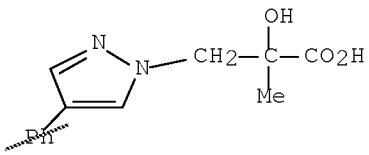
L14 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1994:244826 CAPLUS Full-text
DOCUMENT NUMBER: 120:244826
ORIGINAL REFERENCE NO.: 120:43397a,43400a
TITLE: Wolff-Kishner reduction of 5-methyl- and 6,6-dimethyl-5-hydroxy-4-oxo-3-phenylpyrrolo[1,2-b]pyrazoles
AUTHOR(S): Kuzmenok, N. M.; Zvonok, A. M.
CORPORATE SOURCE: Beloruss. Tekhnol. Inst., Minsk, Belarus
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1993), (10), 1345-8
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



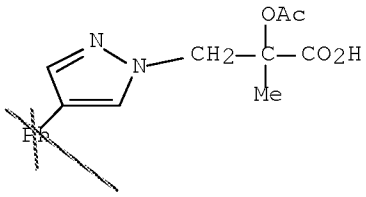
I

AB Wolff-Kishner redn. of the title compds. I (R = H, R1 = Me; R = Me, R1 = H) by hydrazine hydrate in basic media is accompanied by decompn. of the bicyclic skeleton or dehydration depending on the solvent and reaction temps.
IT 127703-13-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and acetylation of)
RN 127703-13-3 CAPLUS

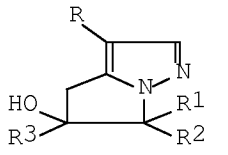
CN 1H-Pyrazole-1-propanoic acid, .alpha.-hydroxy-.alpha.-methyl-4-phenyl-
(CA INDEX NAME)



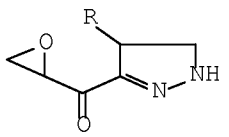
IT 127703-14-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 127703-14-4 CAPLUS
CN 1H-Pyrazole-1-propanoic acid, .alpha.-(acetyloxy)-.alpha.-methyl-4-phenyl-
(CA INDEX NAME)



L14 ANSWER 18 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1990:423753 CAPLUS Full-text
DOCUMENT NUMBER: 113:23753
ORIGINAL REFERENCE NO.: 113:4119a,4122a
TITLE: Synthesis and chemical transformations of 5-hydroxy-4-oxo-3-arylpyrrolidino[1,2-b]pyrazoles
AUTHOR(S): Zvonok, A. M.; Kuz'menok, N. M.; Stanishevskii, L. S.
CORPORATE SOURCE: Nauchno-Issled. Inst. Fiz.-Khim. Probl., Minsk, 220080, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1989), (10), 1391-5
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 113:23753
GI



I



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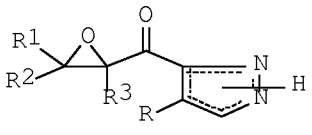
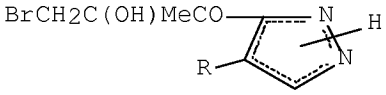


III



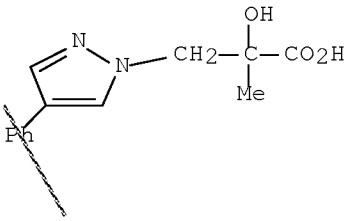
IV

AB Pyrrolopyrazoles I (R = Ph, 4-MeOC6H4, 4-BrC6H4, 3-O2NC6H4, R1 = R2 = H, R3 = Me; R = Ph, R1 = R2 = Me, R3 = H), prepd. from epoxy derivs. II by treatment with NBS or Et3N, by treatment of epoxy derivs. III with HBr, and by cyclization of pyrazoles IV with Et3N, underwent acetylation, redn. by NaBH4, and oxidative and base-catalyzed ring cleavage to give a variety of substituted pyrazoles.

IT 127703-13-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and acetylation of)

RN 127703-13-3 CAPLUS

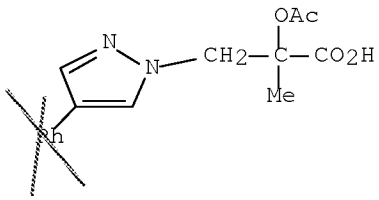
CN 1H-Pyrazole-1-propanoic acid, .alpha.-hydroxy-.alpha.-methyl-4-phenyl- (CA INDEX NAME)



IT 127703-14-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 127703-14-4 CAPLUS

CN 1H-Pyrazole-1-propanoic acid, .alpha.-(acetyloxy)-.alpha.-methyl-4-phenyl- (CA INDEX NAME)



L14 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN

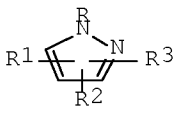
ACCESSION NUMBER: 1979:540839 CAPLUS Full-text

DOCUMENT NUMBER: 91:140839
ORIGINAL REFERENCE NO.: 91:22723a,22726a
TITLE: Pyrazole amides and thioamides
INVENTOR(S): Moon, Malcolm W.; Kornis, Gabriel
PATENT ASSIGNEE(S): Upjohn Co., USA
SOURCE: Can., 115 pp.
CODEN: CAXXA4
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 1053231	A1	19790424	CA 1975-240263	19751124
US 4072498	A	19780207	US 1976-686548	19760514
GB 1510776	A	19780517	GB 1977-9699	19770308
US 4097672	A	19780627	US 1977-795103	19770509
FR 2351104	A2	19771209	FR 1977-14624	19770512
BE 854613	A4	19771114	BE 1977-177558	19770513
US 4111941	A	19780905	US 1977-846179	19771027
US 4111939	A	19780905	US 1977-846180	19771027
US 4113955	A	19780912	US 1977-846158	19771027
US 4113956	A	19780912	US 1977-846159	19771027
US 4115649	A	19780919	US 1977-846181	19771027

PRIORITY APPLN. INFO.: US 1974-524231 A 19741115
US 1976-686548 A 19760514

GI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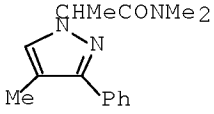
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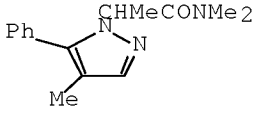
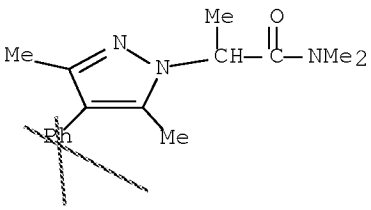

III

AB Herbicidal (no data) pyrazoles I (R = carbamoylalkyl, thiocarbamoylalkyl, attached through .alpha.-C or .beta.-C; R1, R2 = H, alkyl, Ph, halogen, CN, NO2, CF3; R3 = optionally substituted Ph, thienyl, furyl) (.apprx.200 compds.) were prepd. Thus, the Na salt was prepd. from 10.5 g 4-methyl-3-phenylpyrazole and treated with 10 g ClCHMeCONMe2 to give 17.7 g II and 2.4 g III.

IT 59843-47-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 59843-47-9 CAPLUS
CN 1H-Pyrazole-1-acetamide, N,N,.alpha.,3,5-pentamethyl-4-phenyl- (CA INDEX NAME)

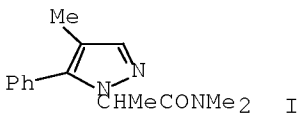


OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)

L14 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1976:446670 CAPLUS Full-text
DOCUMENT NUMBER: 85:46670
ORIGINAL REFERENCE NO.: 85:7591a,7594a
TITLE: Herbicidal substituted pyrazoles
INVENTOR(S): Moon, Malcolm W.; Kornis, Gabriel
PATENT ASSIGNEE(S): Upjohn Co., USA
SOURCE: Ger. Offen., 117 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2550566	A1	19760520	DE 1975-2550566	19751111
ZA 7506627	A	19770525	ZA 1975-6627	19751021
AU 7585957	A	19770428	AU 1975-85957	19751023
GB 1483162	A	19770817	GB 1975-43505	19751023
CH 629364	A5	19820430	CH 1975-14174	19751103
BR 7507364	A	19760810	BR 1975-7364	19751107
BE 835604	A1	19760514	BE 1975-161900	19751114
FR 2324633	A1	19770415	FR 1975-34913	19751114
SU 581838	A3	19771125	SU 1975-2190909	19751114
SU 613722	A3	19780630	SU 1975-2189715	19751114
JP 51082269	A	19760719	JP 1975-137708	19751115
PL 101829	B1	19790228	PL 1975-184782	19751115
PRIORITY APPLN. INFO.:			US 1974-524231 A	19741115

GI



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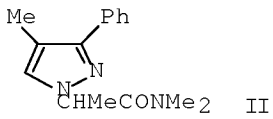
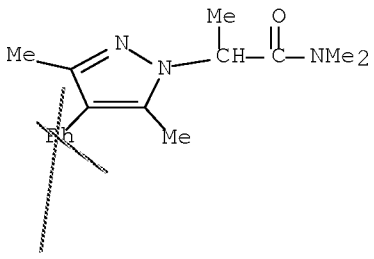


II

AB Pyrazoleacetamides (>150 compds.) such as I and II were prepd. Thus, I and II were obtained by treating 4-methyl-3-phenylpyrazole Na salt with ClCHMeCONMe2.

IT 59843-47-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 59843-47-9 CAPLUS
CN 1H-Pyrazole-1-acetamide, N,N,.alpha.,3,5-pentamethyl-4-phenyl- (CA INDEX NAME)

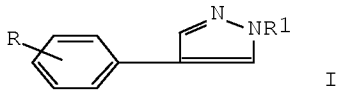


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L14 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1976:180209 CAPLUS Full-text
DOCUMENT NUMBER: 84:180209
ORIGINAL REFERENCE NO.: 84:29207a,29210a
TITLE: 4-Phenyl-1-hydroxyalkylpyrazoles
INVENTOR(S): Hardtmann, Goetz E.
PATENT ASSIGNEE(S): Sandoz-Wander, Inc., USA
SOURCE: U. S. Publ. Pat. Appl. B, 4 pp.
CODEN: USXXDP
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 535437	I5	19760224	US 1974-535437	19741223
US 3997555	A	19761214		
PRIORITY APPLN. INFO.:			US 1974-535437	19741223

GI

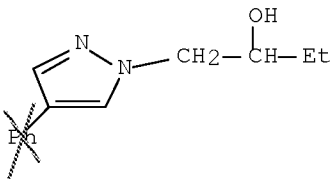


I

AB Pyrazoles [I, R = m-F3C, H, p-MeO, m-Me, m-F, R1 = CH2CH(OH)Et, CH2CH2OH, (CH2)3OH], useful as tranquilizers and muscle-relaxants, were obtained by refluxing R1NHNH2 with Me2NCH:C(C6H4R)CHO in C6H6 2.5 hr.

IT 59198-11-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 59198-11-7 CAPLUS
CN 1H-Pyrazole-1-ethanol, .alpha.-ethyl-4-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L14 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1971:125554 CAPLUS Full-text
DOCUMENT NUMBER: 74:125554
ORIGINAL REFERENCE NO.: 74:20283a,20286a
TITLE: Synthesis of pyrroles, pyrazolines, and pyrazoles via bis-en-hydrazines
AUTHOR(S): Fritz, Helmut; Uhrhan, Paul
CORPORATE SOURCE: Inst. Org. Chem., Univ. Frankfurt, Frankfurt, Fed. Rep. Ger.
SOURCE: Justus Liebigs Annalen der Chemie (1971), 744, 81-7
CODEN: JLACBF; ISSN: 0075-4617
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 74:125554

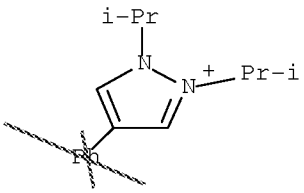
AB Cyclic and open-chain carbonyl compds. reacted with MeNHNHMe to yield the intermediate bis-ene-hydrazines RCH:CR1NMeNMeCR1:CHR (sic) (I) (where R = org. substituent). On thermolysis or acid catalysis of I, the corresponding N-methylpyrroles (II) were formed. Similar reaction of MeNHNH2 also led to the formation of II. In some cases, pyrazolines were formed in a competitive reaction. In the presence of suitable leaving group effects, the pyrazolines were converted into pyrazole or pyrazolium systems by .beta.-elimination.

IT 31703-69-2P 31703-70-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 31703-69-2 CAPLUS
CN Pyrazolium, 1,2-diisopropyl-4-phenyl-, picrate (8CI) (CA INDEX NAME)

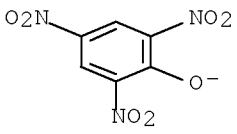
CM 1

CRN 46814-57-7
CMF C15 H21 N2

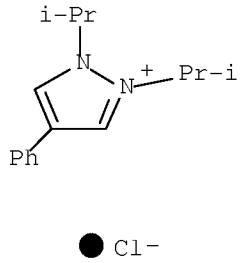


CM 2

CRN 14798-26-6
CMF C6 H2 N3 O7



RN 31703-70-5 CAPLUS
CN 1H-Pyrazolium, 1,2-bis(1-methylethyl)-4-phenyl-, chloride (1:1) (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

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Executing the logoff script...

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FULL ESTIMATED COST	124.58	480.76

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-18.04	-18.04

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 11:38:54 ON 17 DEC 2009